FOR OFFICIAL USE ONLY

U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

Examiner # (Mandatory): _____ Requester's Full Name: _____

Art Unit _____ Location (Bldg/Room#): _____ Phone (circle 305 306 308) _____

Serial Number: _____ Results Format Preferred (circle): PAPER DISK E-MAIL

Title of Invention _____

Inventors (please provide full names): _____

meg

Earliest Priority Date: _____

Keywords (include any known synonyms registry numbers, explanation of initialisms):

See attached

Search Topic:
Please write detailed statement of the search topic, and the concept of the invention. Describe as specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples of relevant citations, authors, etc., if known. You may include a copy of the abstract and the broadcast or most relevant claim(s).

Point of Contact:
Thomas G. Larson, Ph.D.
703-308-7309
CM1, Rm. 6 B 01

STAFF USE ONLY

Searcher: _____
Searcher Phone #: _____
Searcher Location: _____
Date Picked Up: 12/30
Date Completed: 1/3/03
Clerical Prep Time: 60
Terminal Time: 325
Number of Databases: _____

Type of Search

_____	N.A. Sequence
_____	A.A. Sequence
2	Structure (#)
_____	Bibliographic
_____	Litigation1
_____	Fulltext
_____	Procurement
_____	Other

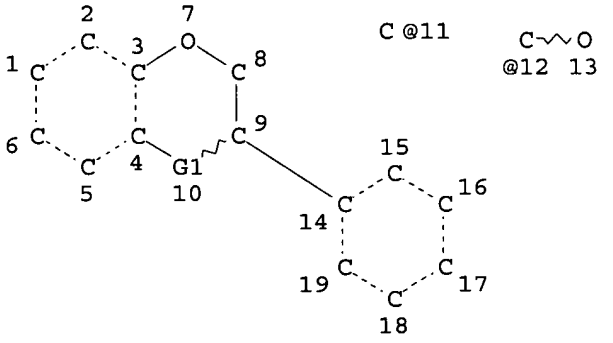
Vendors (include cost where applicable)

725	STN
_____	Questel/Orbit
_____	Lexis/Nexis
_____	WWW/Internet
_____	In-house sequence systems (list)
_____	Dialog
_____	Dr. Link
_____	Westlaw
_____	Other (specify)

PTO-1590 (2-99)

Results for structure (II)


```
=> FIL REG
FILE 'REGISTRY' ENTERED AT 16:35:53 ON 03 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    2 JAN 2003  HIGHEST RN 478001-04-6
DICTIONARY FILE UPDATES:   2 JAN 2003  HIGHEST RN 478001-04-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d que l11
L1                SCR 1133
L2                SCR 1135
L3                SCR 1044
L4                SCR 2050
L5                SCR 2043
L6                SCR 1918
L7                STR
```



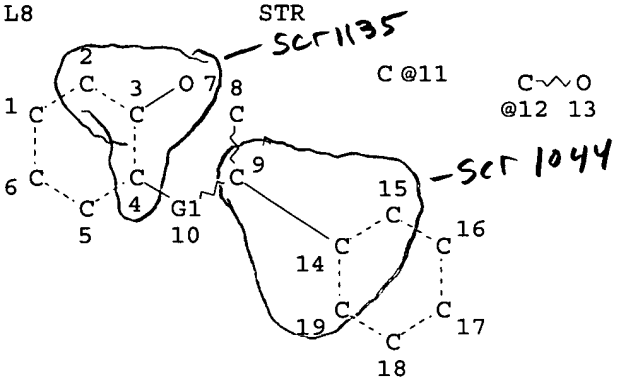
see results for structure I for explanation.

```
VAR G1=11-4 11-9/12-4 12-9
NODE ATTRIBUTES:
CONNECT IS E2  RC AT   2
CONNECT IS E2  RC AT   5
CONNECT IS E2  RC AT   8
CONNECT IS E3  RC AT   9
CONNECT IS E2  RC AT  11
CONNECT IS E3  RC AT  12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  19
```

Searched by Thom Larson, STIC, 308-7309

Point of Contact:
Thomas G. Larson, Ph.D.
703-308-7309
CM1, Rm. 6 B 01

STEREO ATTRIBUTES: NONE
L8 STR



Initial structure for compound II - bond 8-9 is undefined (un) so that both single and double bonds will be picked up, R_1-R_4 are left undefined.

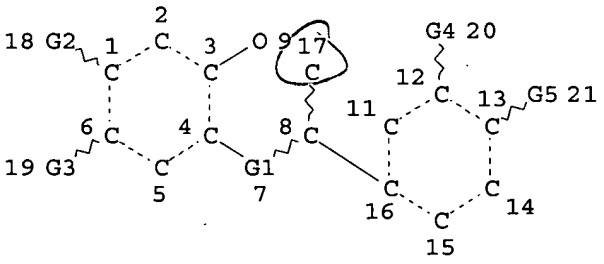
VAR G1=11-4 11-9/12-4 12-9
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 5
CONNECT IS E2 RC AT 8
CONNECT IS E3 RC AT 9
CONNECT IS E2 RC AT 11
CONNECT IS E3 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L9 (1531) SEA FILE=REGISTRY SSS FUL (L7 OR L8) AND ((L1 OR L2) AND L3) NOT (L4 OR L5 OR L6)

} initial answer set - see results for structure I for details

L10 STR



This structure is the same as L8 but refines the answer set by introducing R_1-R_4 to H or -O- (as in OH or OMe). Also, C @ 17 is limited to having only H substituents.

R_3 VAR G1=22-4 22-8/23-4 23-8
R_4 VAR G2=H/O
R_2 VAR G3=H/O
R_1 VAR G4=H/O
VAR G5=H/O
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 5
CONNECT IS E3 RC AT 8
CONNECT IS E2 RC AT 11
CONNECT IS E2 RC AT 14
CONNECT IS E2 RC AT 15
CONNECT IS E1 RC AT 17

CONNECT IS E2 RC AT 22
CONNECT IS E3 RC AT 23
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
L11 0 SEA FILE=REGISTRY SUB=L9 SSS FUL L10

Search answer set L9 with structure L10 — structure L10 is still broader than compound (II) — so it should have picked up any similar structures.

Results for structure (I).


```
=> file reg hcaplus
FILE 'REGISTRY' ENTERED AT 15:35:12 ON 03 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

FILE 'HCAPLUS' ENTERED AT 15:35:12 ON 03 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

=> d que l39
L1                SCR 1133
L2                SCR 1135
L3                SCR 1044
L4                SCR 2050
L5                SCR 2043
L6                SCR 1918
L7                STR
```

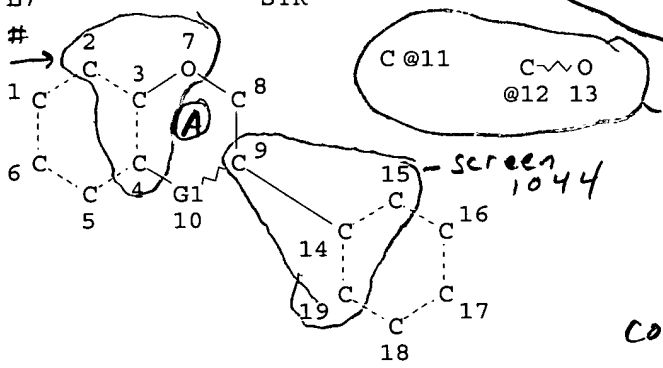
This screen is for the configuration of the C @ # 3 in L7

This screen is for same configuration but the C-O bond is a chain bond - see L8

This screen is for the configuration of the C @ #4 in both L3 & L8

2050 - alloys
2043 - metals
1918 - polymers

screen # 1133

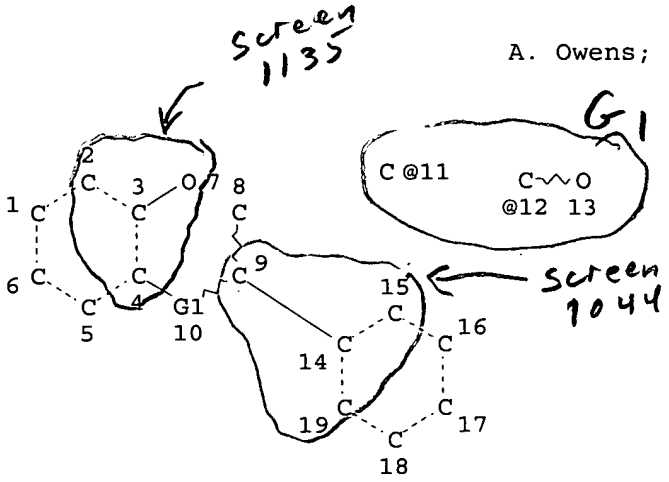


screen 1044

This structure looks for compounds like I. G_1 can have C11 or C12 in the ring allowing ring A to have a -H, -OH, or =O moiety attached to ring @ G_1. The undefined bond (~) @ G_1 - C9 allows that bond to be either a single or double bond. R_1 - R_4 are left open and will be defined later.

```
VAR G1=11-4 11-9/12-4 12-9
NODE ATTRIBUTES:
CONNECT IS E2  RC AT   2
CONNECT IS E2  RC AT   5
CONNECT IS E2  RC AT   8
CONNECT IS E3  RC AT   9
CONNECT IS E2  RC AT  11
CONNECT IS E3  RC AT  12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  19

STEREO ATTRIBUTES: NONE
L8                STR
```


Point of Contact:
Thomas G. Larson, Ph.D.
703-308-7309
CM1, Rm. 6 B 01



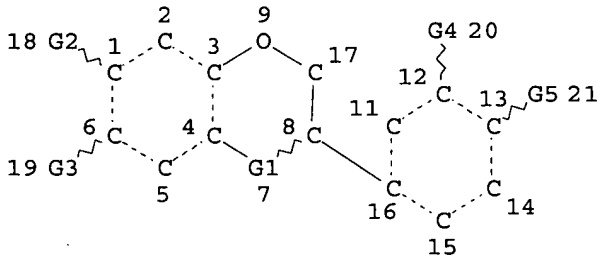
This searches for structure II and will be discussed in the results for that structure.

VAR G1=11-4 11-9/12-4 12-9
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 5
CONNECT IS E2 RC AT 8
CONNECT IS E3 RC AT 9
CONNECT IS E2 RC AT 11
CONNECT IS E3 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L9 (1531)SEA FILE=REGISTRY SSS FUL (L7 OR L8) AND ((L1 OR L2) AND L3) NOT (L4 OR L5 OR L6) — not metal or alloy or polymer
L10 STR

structure I, structure II, scr 1133, scr 1135, scr 1044 → initial answer set — combines structures I & II



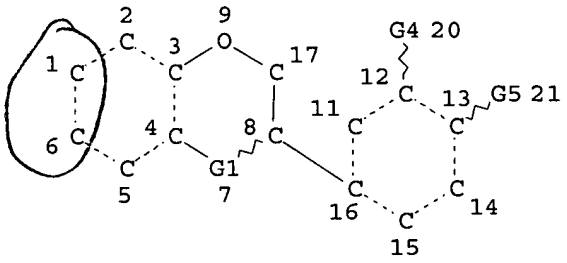
This structure is the same as L7, but refines the answer set by defining R_1 - R_4 of structure I

VAR G1=22-4 22-8/23-4 23-8
R_3 VAR G2=H/OH/MEO
R_4 VAR G3=H/OH/MEO
R_2 VAR G4=H/OH/MEO
R_1 VAR G5=H/OH/MEO
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 5
CONNECT IS E3 RC AT 8
CONNECT IS E2 RC AT 11
CONNECT IS E2 RC AT 14
CONNECT IS E2 RC AT 15
CONNECT IS E2 RC AT 17
CONNECT IS E2 RC AT 22
CONNECT IS E3 RC AT 23

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
L11 STR

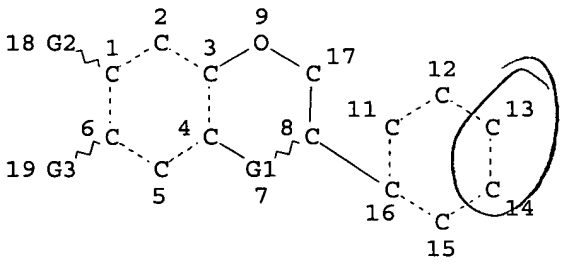


This structure represents the special case where R_3 & R_4 are both H — see lines 9-10 claim 1.

VAR G1=22-4 22-8/23-4 23-8
VAR G4=H/OH/MEO
VAR G5=H/OH/MEO
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 1
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 5
CONNECT IS E2 RC AT 6
CONNECT IS E3 RC AT 8
CONNECT IS E2 RC AT 11
CONNECT IS E2 RC AT 14
CONNECT IS E2 RC AT 15
CONNECT IS E2 RC AT 17
CONNECT IS E2 RC AT 22
CONNECT IS E3 RC AT 23
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE
L12 STR



C @22 C~O @23 24

R_1 & R_2 are both H — lines 7-8 of claim 1.

VAR G1=22-4 22-8/23-4 23-8
VAR G2=H/OH/MEO
VAR G3=H/OH/MEO
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2

```
CONNECT IS E2  RC AT   5
CONNECT IS E3  RC AT   8
CONNECT IS E2  RC AT  11
CONNECT IS E2  RC AT  13
CONNECT IS E2  RC AT  14
CONNECT IS E2  RC AT  15
CONNECT IS E2  RC AT  17
CONNECT IS E2  RC AT  22
CONNECT IS E3  RC AT  23
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  21

STEREO ATTRIBUTES: NONE
L13 (        91)SEA FILE=REGISTRY SUB=L9 SSS FUL L10 NOT (L11 OR L12)
L14 (         1)SEA FILE=REGISTRY ABB=ON  PLU=ON  531-95-3
L15          90 SEA FILE=REGISTRY ABB=ON  PLU=ON  L13 NOT L14
L35          16 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15 (L) THU/RL
L36          26 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15 (L) BAC/RL
L37          57 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15 (L) SPN/RL
L38          83 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L35 OR L36 OR L37
L39          59 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38 NOT PY>=1999
```

search answer set L9 for refined structure L10 but not special cases L11 or L12.

This answer set gave 384 hits when crossed to HCAPLUS

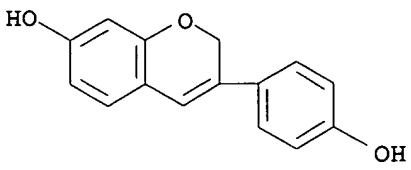
Removing this one registry # reduced the hits to 165

Search HCAPLUS for most relevant hits using hits from Registry — THU/RL: Therapeutic use BAC/RL: Biological activity SPN/RL: Synthetic preparation

narrow further by date to get a reasonable # to print out.

```
=> D IBIB ABS HITSTR 139 1-59

L39  ANSWER 1 OF 59  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         1999:30509  HCAPLUS
DOCUMENT NUMBER:          130:234644
TITLE:                    Antioxidants from Lespedeza homoloba
AUTHOR(S):                Miyase, T.; Sano, M.; Nakai, H.; Muraoka, M.; Yoshino,
                          K.; Nishihara, Y.; Tanai, J.
CORPORATE SOURCE:         School of Pharmaceutical Sciences, University of
                          Shizuoka, Shizuoka, 422-8002, Japan
SOURCE:                   International Congress Series (1998), 1157(Towards
                          Natural Medicine Research in the 21st Century),
                          285-293
                          CODEN: EXMDA4; ISSN: 0531-5131
PUBLISHER:                Elsevier Science B.V.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Eight new and 3 previously isolated isoflavanoids were obtained from the
     methanolic exts. of the stems of Lespedeza homoloba and their structures
     confirmed via NMR data.  These isoflavanoids were tested for their
     antioxidative activity against lipid peroxidn. in rat brain homogenate and
     detd. that those compds. with the strongest activity were complexes
     composed of 2-arylbenzofuran and pterocarp-6a-en.  Iron-chelating and
     superoxide anion radical scavenging activities of these isoflavanoids were
     measured.
IT   81267-65-4P, Haginin E
     RL: BAC (Biological activity or effector, except adverse); BOC
     (Biological occurrence); BSU (Biological study, unclassified); PUR
     (Purification or recovery); BIOL (Biological study); OCCU (Occurrence);
     PREP (Preparation)
        (isolation of lespedezol isoflavanoid antioxidants from Lespedeza
        homoloba)
RN   81267-65-4  HCAPLUS
```

CN 2H-1-Benzopyran-7-ol, 3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



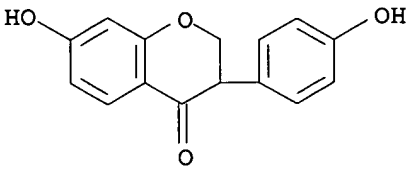
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 2 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:554767 HCAPLUS
DOCUMENT NUMBER: 129:269970
TITLE: Antioxidant activities of isoflavones and their biological metabolites in a liposomal system
AUTHOR(S): Arora, Arti; Nair, Muraleedharan G.; Strasburg, Gale M.
CORPORATE SOURCE: Department of Food Science and Human Nutrition, Michigan State University, East Lansing, MI, 48824, USA
SOURCE: Archives of Biochemistry and Biophysics (1998), 356(2), 133-141
CODEN: ABBIA4; ISSN: 0003-9861
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English

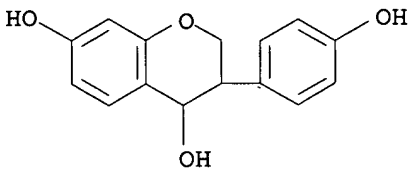
AB Genistein and daidzein, the two major soy isoflavones, principally occur in nature as their glycosylated or methoxylated derivs., which are cleaved in the large intestine to yield the free aglycons and further metabolites. The objective of this study was to compare the antioxidant activities of genistein and daidzein with their glycosylated and methoxylated derivs. and also those of their human metabolites. The abilities of these compds. to inhibit lipid peroxidn. in a liposomal system were evaluated using fluorescence spectroscopy, and structural criteria that enhance antioxidant activity were established. The peroxidn. initiators employed in the study were Fe(II) and Fe(III) metal ions and aq.-phase, azo-derived peroxyl radicals. Both the parent isoflavonoids and their metabolites were more effective at suppressing metal-ion-induced peroxidns. than the peroxyl-radical-induced peroxidn. Antioxidant activities for the isoflavone metabolites were comparable to or superior to those for the parent compds. Equol and its 4-hydroxy and 5-hydroxy derivs. were the most potent antioxidants in the study, suggesting that absence of the 2,3-double bond and the 4-oxo group on the isoflavone nucleus enhances antioxidant activity. Addnl., the no. and position of hydroxyl groups were detg. factors for isoflavonoid antioxidant activity, with hydroxyl substitution being of utmost importance at the C-4' position, of moderate importance at the C-5 position, and of little significance at the C-7 position. (c) 1998 Academic Press.

IT **17238-05-0 175089-66-4**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antioxidant activities of isoflavones and their biol. metabolites in a liposomal system)

RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 175089-66-4 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



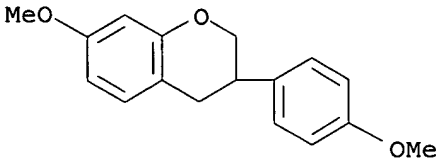
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 3 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:543963 HCAPLUS
DOCUMENT NUMBER: 129:275727
TITLE: The direct synthesis of isoflavans via .alpha.-alkylation of phenylacetates
AUTHOR(S): Versteeg, Mariejie; Bezuidenhoudt, Barend C. B.; Ferreira, Daneel
CORPORATE SOURCE: Dep. Chem., Univ. Orange Free State, Bloemfontein, 9300, S. Afr.
SOURCE: Heterocycles (1998), 48(7), 1373-1394
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:275727

AB Deprotonation of oxygenated phenylacetates and quenching of the enolates with oxygenated benzylic electrophiles, afforded 2,3-diarylpropanoates which served as precursors to the isoflavans following consecutive redn. and cyclization steps. E.g., PhCH2CO2Me was alkylated with 2-(methoxymethoxy)benzyl bromide using BuLi and N-(isopropyl)cyclohexylamine in THF to form 2-(MeOCH2O)C6H4CH2CH(CO2Me)Ph, which subsequently underwent carboxylate redn. with LiAlH4 in Et2O, O deprotection with HCl, and cyclization with PPh3/DEAD in THF to give isoflavan with 87% yield for the cyclization step. When the cyclization step was carried out using PTSA in benzene, isoflavan was formed in 28% yield along with an equal yield of 2-benzyl-2,3-dihydrobenzofuran.

IT **4366-35-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(synthesis of isoflavans via .alpha.-alkylation of phenylacetates)

RN 4366-35-2 HCAPLUS
CN 2H-1-Benzopyran, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

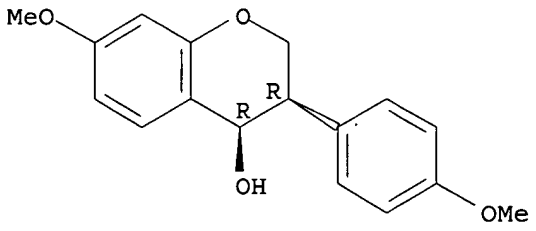
L39 ANSWER 4 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:256815 HCAPLUS
DOCUMENT NUMBER: 129:54205
TITLE: Diastereoselectivity of various routes to isoflavan-4-ols (3-phenyl-4-chromanols)
AUTHOR(S): Chidiak, Henry; Kirkiacharyan, S.
CORPORATE SOURCE: Lab. Chim. Ther. Fac. Pharm., Univ. Paris, Paris, Fr.
SOURCE: Khimicheskii Zhurnal Armenii (1996), 49(1-3), 94-104
CODEN: KZARF3
PUBLISHER: Izdatel'stvo Gitutyun NAN Respubliki Armenii
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The redn. of isoflavan-4-ones (3-phenyl-4-chromanones) by nucleophilic hydrides (sodium borohydride, lithium aluminum tri-tert-butoxyhydride, lithium tri-sec-butylborohydride) leads to mixts. of cis and trans diastereoisomers of isoflavan-4-ols. Redn. by electrophilic hydrides (borane-THF, bis-tert-butylthioethane diborane, or 9-borabicyclo[3.3.1]nonane) is stereoselective and forms cis diastereoisomers in excellent yields. Hydroboration, followed by alk. hydroperoxide oxidn., of 3-phenyl-4-hydroxycoumarins is a stereoselective route to trans diastereoisomers of isoflavan-4-ols.

IT **6228-91-7P 20986-82-7P 208708-06-9P 208708-07-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(diastereoselectivity of various routes to isoflavan-4-ols)

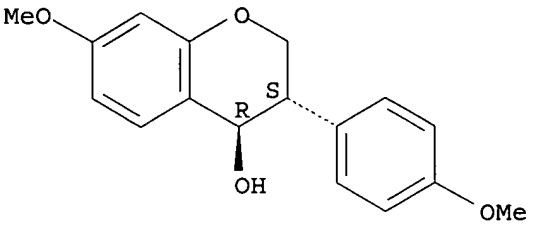
RN 6228-91-7 HCAPLUS
CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



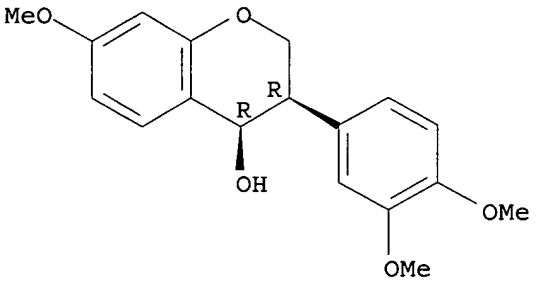
RN 20986-82-7 HCAPLUS
CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



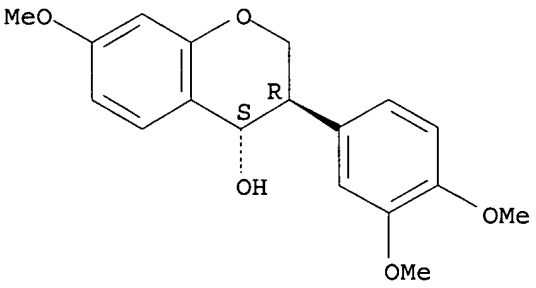
RN 208708-06-9 HCAPLUS
CN 2H-1-Benzopyran-4-ol, 3-(3,4-dimethoxyphenyl)-3,4-dihydro-7-methoxy-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 208708-07-0 HCAPLUS
CN 2H-1-Benzopyran-4-ol, 3-(3,4-dimethoxyphenyl)-3,4-dihydro-7-methoxy-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



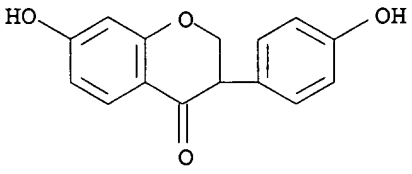
L39 ANSWER 5 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:130933 HCAPLUS
DOCUMENT NUMBER: 128:204711
TITLE: Synthesis of novel mammalian metabolites of the isoflavonoid phytoestrogens daidzein and genistein
AUTHOR(S): Wahala, Kristiina; Salakka, Auli; Adlercreutz, Herman
CORPORATE SOURCE: Department of Chemistry, Organic Chemistry Laboratory, University of Helsinki, FIN-00014, Finland
SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1998), 217(3), 293-299
CODEN: PSEBAA; ISSN: 0037-9727
PUBLISHER: Blackwell Science, Inc.

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of novel mammalian metabolites of dietary isoflavones, dihydrodaidzein (4',7-dihydroxyisoflavanone), dihydrogenistein (4',5,7-trihydroxy-isoflavanone), 6'-hydroxy-O-demethylangolensin [1-(2,4,6-trihydroxyphenyl)-2-(4-hydroxyphenyl)propan-1-one], and cis- and trans-4',7-dihydroxylsoflavan-4-ols is described, and their characteristics by phys. and chem. consts. given for the first time.

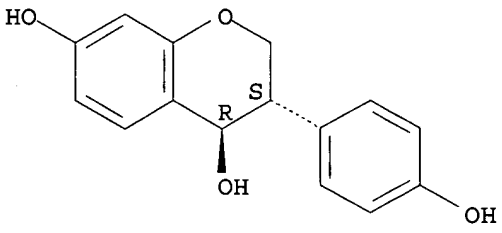
IT **17238-05-0P 168207-15-6P 168207-16-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(synthesis of novel mammalian metabolites of isoflavonoid phytoestrogens daidzein and genistein)

RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



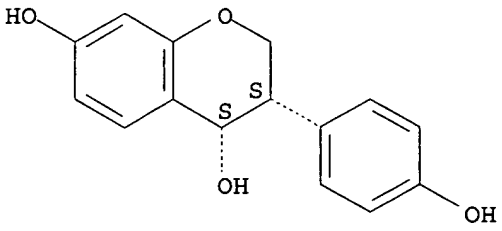
RN 168207-15-6 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 168207-16-7 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



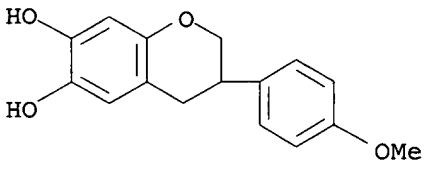
L39 ANSWER 6 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:20731 HCAPLUS
DOCUMENT NUMBER: 128:164027
TITLE: Isoflavonoids as inhibitors of lipid peroxidation and quenchers of singlet oxygen
AUTHOR(S): Briviba, Karlis; Sies, Helmut; Sepulveda-Boza, Silvia; Zilliken, Friedrich W.
CORPORATE SOURCE: Heinrich Heine University, Dusseldorf, Germany
SOURCE: Antioxidants in Health and Disease (1998), 7(Flavonoids in Health and Disease), 295-302
CODEN: AHDIEQ
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This report examines the inhibition of microsomal lipid peroxidn. and the ability of singlet oxygen quenching of some new isoflavones and isoflavans and compares the antioxidant properties of these isoflavonoids with established antioxidants.

IT **76397-87-0**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(isoflavonoids as inhibitors of lipid peroxidn. and quenchers of singlet oxygen)

RN 76397-87-0 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 7 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:13303 HCAPLUS
DOCUMENT NUMBER: 128:114255
TITLE: Identification of isoflavonoids in beer
AUTHOR(S): Lapcik, Oldrich; Hill, Martin; Hampl, Richard; Wahala, Kristiina; Adlercreutz, Herman
CORPORATE SOURCE: Institute of Endocrinology, Prague, 116 94/1, Czech Rep.
SOURCE: Steroids (1998), 63(1), 14-20
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

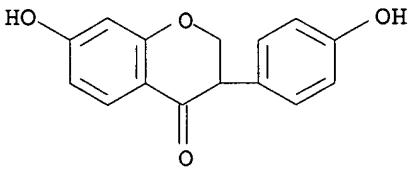
AB The isoflavonoids, genistein (4',5,7-trihydroxyisoflavone), biochanin A (5,7-dihydroxy-4'-methoxyisoflavone), daidzein (4',7-dihydroxyisoflavone), and formononetin (7-hydroxy-4'-methoxyisoflavone) are supposed to be health-promoting dietary factors of plant origin. They are particularly abundant in seeds and other parts of many plant species belonging to Leguminosae. The most popular source of isoflavonoids in human diet is soy. Here, evidence is presented that isoflavonoids are regularly found in beer. Di-Et ether exts. of beer were fractionated on thin-layer chromatog.-silica, (straight phase) and rechromatographed using a reversed phase high-performance liq. chromatog. octadecylsilica column. The fractions were analyzed by two recently developed RIAs, the first of them

being specific for daidzein/formononetin and the second one specific for genistein/biochanin A. The immunoreactivity was found only in fractions with the mobility corresponding to the positions of stds. on control chromatograms. Addnl., 26 samples of bottled beer were analyzed for isoflavonoid content using the combination of reversed phase high-performance liq. chromatog. and RIA. The sum of the four isoflavonoids ranged from 1.26 to 29 nmol/L in individual beers. Formononetin was the major isoflavonoid (0.19-14.99 nmol/L), whereas the concn. of daidzein was several times lower (0.08-2.5 nmol/L). Genistein and biochanin A concns. were comparable, ranging from 0.169-6.74 nmol/L and from 0.820-4.84 nmol/L for genistein and biochanin A, resp. It is concluded that beer contains significant amts. of biol. active isoflavonoid phytoestrogens.

IT **17238-05-0**
RL: **BAC (Biological activity or effector, except adverse)**; BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(identification of isoflavonoids in beer)

RN 17238-05-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 8 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:658532 HCAPLUS

DOCUMENT NUMBER: 127:307275

TITLE: The Synthesis, Structure and Anticancer Activity of cis- and trans-4',7-Dihydroxyisoflavan-4-ols

AUTHOR(S): Waehaelae, Kristiina; Koskimies, Jorma K.; Mesilaakso, Markku; Salakka, Auli K.; Leino, Tero K.; Adlercreutz, Herman

CORPORATE SOURCE: Organic Chemistry Laboratory, University of Helsinki, Helsinki, FIN-00014, Finland

SOURCE: Journal of Organic Chemistry (1997), 62(22), 7690-7693
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

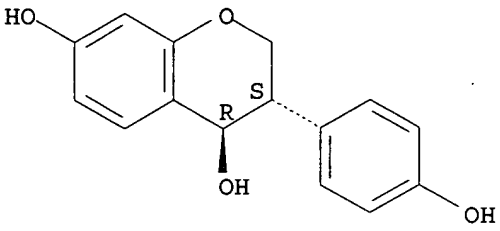
AB Cis-4',7-Dihydroxyisoflavan-4-ol (4) and trans-4',7-dihydroxyisoflavan-4-ol (5), two proposed metabolites of daidzein (4',7-dihydroxyisoflavone), have been synthesized and fully characterized for the first time. The vicinal coupling consts. of the pyran ring protons are compatible with a half-chair conformation. The cis isomer is anancomeric while the trans isomer consists of a 68:32 mixt. of two ring inversion conformers. Mol. mech. calcns. are in agreement with the half-chair conformation of the pyran ring and suggest that the cis isomer is biased because of an unfavorable gauche interaction of the equatorial hydroxyl and the axial Ph group. The isoflavanols 4 and 5 are comparable to genistein (4',5,7-trihydroxyisoflavone) in antitumor activity against human prostate cancer cells.

IT **168207-15-6P 168207-16-7P**

RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PRP (Properties); **SPN (Synthetic preparation)**; BIOL (Biological study); PREP (Preparation)
(prepn., conformation, and anticancer activity of dihydroxyisoflavanols)

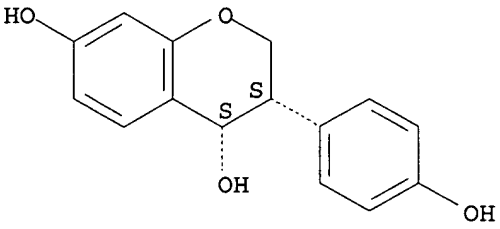
RN 168207-15-6 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



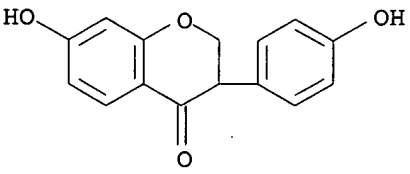
RN 168207-16-7 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **17238-05-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(prepn., conformation, and anticancer activity of dihydroxyisoflavanols)

RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 9 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:198614 HCAPLUS
DOCUMENT NUMBER: 126:211966
TITLE: Deuteration of isoflavonoids

AUTHOR(S): Wahala, Kristiina
CORPORATE SOURCE: Org. Chem. Lab., Univ. Helsinki, FIN-00014, Finland
SOURCE: Polyphenols Actualites (1997), 16, 5-8
CODEN: POACF4; ISSN: 0987-7819
PUBLISHER: Groupe Polyphenols
DOCUMENT TYPE: Journal
LANGUAGE: English

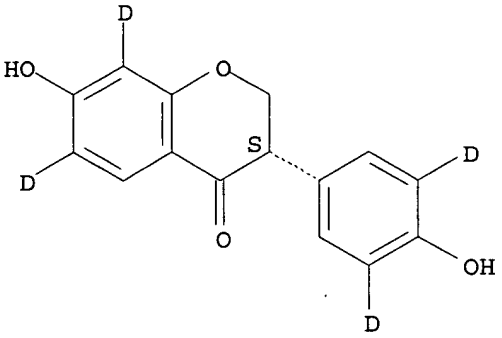
AB Methods are described for the synthesis of deuterium-labeled biol. active isoflavonoids present in human diet and fluids. These compds. receive increasing attention due to their anticancer properties. The hydrogen-deuterium exchange at arom. rings was carried out with PBr3 or NaOD in deuterium oxide or labeled trifluoroacetic acid. The isotopic purity and position of deuterium labels are discussed.

IT **187960-07-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(deuteration of isoflavonoids)

RN 187960-07-2 HCAPLUS

CN 4H-1-Benzopyran-4-one-6,8-d2, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl-3,5-d2)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



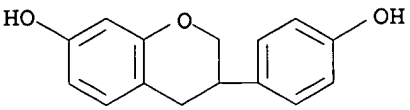
L39 ANSWER 10 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:117690 HCAPLUS
DOCUMENT NUMBER: 124:260636
TITLE: Metabolites of daidzein and genistein and their biological activities
AUTHOR(S): Chang, Yu-Chen; Nair, Muraleedharan G.; Nitiss, John L.
CORPORATE SOURCE: Bioactive Natural Product Lab., Michigan State Univ., East Lansing, MI, 48824, USA
SOURCE: Journal of Natural Products (1995), 58(12), 1901-5
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Society of Pharmacognosy
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A no. of metabolites of daidzein and genistein have been synthesized and their biol. activities detd. Equol, 5,7,4'-trihydroxyisoflavan, 4,7,4'-trihydroxyisoflavan, dihydrodaidzein, and dihydrogenistein were synthesized either from daidzein or genistein by hydrogenation. During acetylation and nmr expts., dihydrogenistein was converted to a novel enol intermediate. Antifungal, antibacterial, mosquitocidal, nematocidal, and topoisomerase inhibition activities of these compds. were evaluated, with equol being the most active of the compds. tested against topoisomerase I.

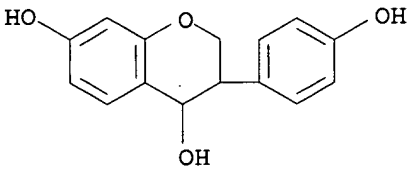
IT **94105-90-5P 175089-66-4P**

RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); **SPN (Synthetic preparation)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and biol. activities of metabolites of daidzein and genistein)

RN 94105-90-5 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

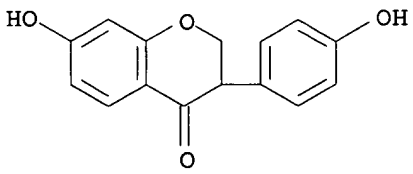


RN 175089-66-4 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



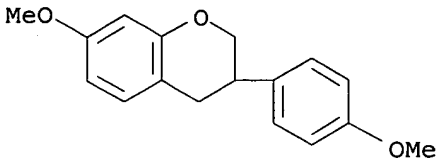
IT **17238-05-0P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; BIOL (Biological study); PREP (Preparation)
(prepn. and biol. activities of metabolites of daidzein and genistein)

RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IT **4366-35-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. and biol. activities of metabolites of daidzein and genistein)

RN 4366-35-2 HCAPLUS
CN 2H-1-Benzopyran, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



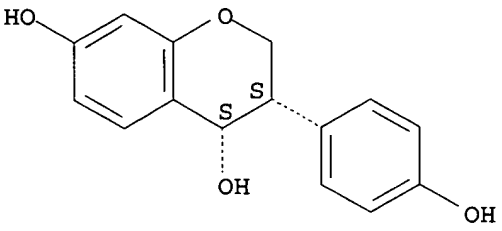
L39 ANSWER 11 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:787564 HCAPLUS
DOCUMENT NUMBER: 123:226958
TITLE: A urinary profile study of dietary phytoestrogens. The identification and mode of metabolism of new isoflavonoids
AUTHOR(S): Joannou, G. E.; Kelly, G. E.; Reeder, A. Y.; Waring, M.; Nelson, C.
CORPORATE SOURCE: Department of Metabolic Mass Spectrometry, Royal Prince Alfred Hospital, Sydney, 2050, Australia
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1995), 54(3/4), 167-84
CODEN: JSBBEZ; ISSN: 0960-0760
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The metabolic fate of the dietary isoflavones daidzein and genistein was investigated in human volunteers challenged with soya. Urinary diphenols, isolated by partition chromatog. on Sephadex LH-20, were characterized and identified by profile capillary gas chromatog. (GC) and electron ionization mass spectrometry (GC-EIMS) anal. of the trimethylsilyl ether (TMS) derivs. Novel isoflavonic phytoestrogens found in the urine of volunteers were those of tetrahydrodaidzein, dihydrogenistein, 6'-hydroxy-O-demethylangolensin and 2-dehydro-O-demethylangolensin. Other known diphenols identified were those of equol, dihydrodaidzein, O-demethylangolensin, daidzein, genistein, glycitein, and the lignan enterolactone. Two other urinary isomers with a fragmentation pattern closely resembling that of the persilylated TMS ethers of cis/trans-isomers of tetrahydrodaidzein, were characterized based on the elucidation of fragments assocd. with the loss of a nonphenolic-OTMS functional group in ring-C. These are fragments presented in the persilylated mass spectra of isoflavan-4-ols and isoflav-3-ene-4-ols, demonstrated here by a combination of simple and tandem mass spectrometry study of the deuterated persilylated TMS ethers of dihydrodaidzein. In a similar study the authors also present the data on the structural identification and fragment elucidation of the keto/enol tautomers of the TMS ether derivs. of the dihydro derivs. of daidzein and genistein, obsd. in the urine of volunteers and considered probable products of the derivatization process. Finally, the GC and GC-MS data of two unknown isoflavonoids and that of a lignan-like compd. are presented together with those of dihydrodaidzein, dihydrogenistein, tetrahydrodaidzein and 2-dehydro-O-demethylangolensin. The latter four were obtained here as products of small scale chem. synthesis in a preliminary study on the tentative identification of urinary isoflavonoids in human volunteers challenged with soya.

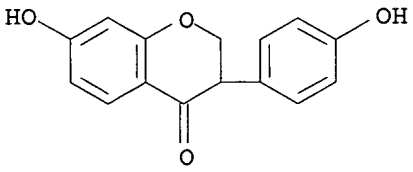
IT **168207-16-7P**
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); **SPN (Synthetic preparation)**; BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(mass spectra of synthesized isoflavonoids)

RN 168207-16-7 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

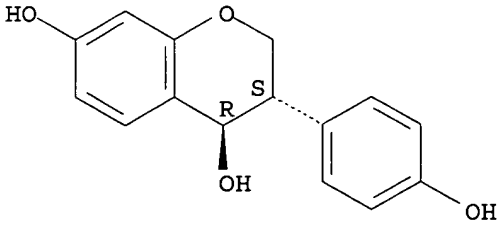


IT **17238-05-0P 168207-15-6P 168207-18-9P**
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); **SPN (Synthetic preparation)**; BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(urinary metabolites of dietary soya isoflavones and mass spectra of synthesized compds.)
RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

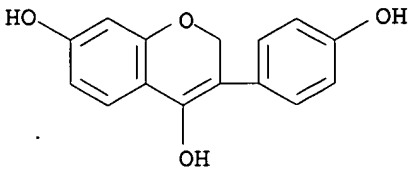


RN 168207-15-6 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 168207-18-9 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

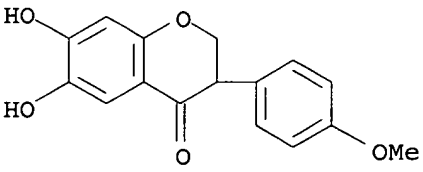


L39 ANSWER 12 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:359059 HCAPLUS
DOCUMENT NUMBER: 122:156104
TITLE: Structure-activity relationships among isoflavonoids with regard to their antifungal properties
AUTHOR(S): Weidenboerner, Martin; Jha, Hem Chandra
CORPORATE SOURCE: Institut fur Lebensmitteltechnologie, Universitat Bonn, Bonn, 53117, Germany
SOURCE: Mycological Research (1994), 98(12), 1376-8
CODEN: MYCRER; ISSN: 0953-7562
DOCUMENT TYPE: Journal
LANGUAGE: English

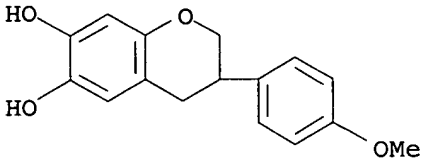
AB In order to establish a structure-activity relationship in the class of isoflavonoids, 16 differently substituted isoflavonoids were tested against Alternaria alternata, Cladosporium herbarum, Fusarium oxysporum and Trichoderma harzianum. The isoflavanones, 6,7-dihydroxy-4'methoxy- and 7-hydroxy-8,4'-dimethylisoflavanone, showed highest antifungal activity in the case of C. herbarum as test fungus. The unreduced structure of the isoflavones has less inhibitory effect on the growth of the test fungi, whereas the completely reduced isoflavones, i.e., the isoflavans, showed only a very weak activity.

IT **76397-85-8 76397-87-0**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(structure-activity relationships among isoflavonoids with regard to their antifungal properties)

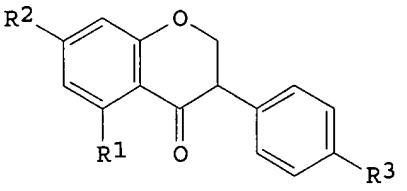
RN 76397-85-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6,7-dihydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



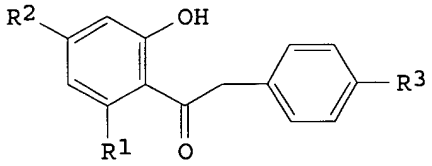
RN 76397-87-0 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 13 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:482765 HCAPLUS
DOCUMENT NUMBER: 121:82765
TITLE: A new facile synthesis of isoflavanones
AUTHOR(S): Bhaskar, T.; Ravichandran, R.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, 600 025, India
SOURCE: Chemical & Environmental Research (1992), 1(2), 107-8
CODEN: CEREEH; ISSN: 0971-2151
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:82765
GI



I



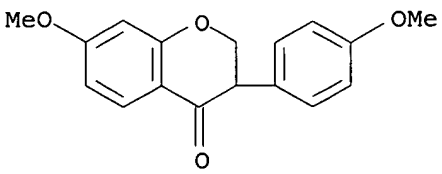
II

AB Isoflavanones I (R1 = R3 = H, R2 = OMe; R1 = R2 = OMe, R3 = H; R1 = H, R2 = R3 = OMe; R1 = R2 = R3 = OMe) were prepd. by reacting malononitrile with 2-hydroxydesoxybenzoins II.

IT **15236-11-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 15236-11-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 14 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:217185 HCAPLUS
DOCUMENT NUMBER: 120:217185
TITLE: Organolead-mediated arylation of allyl

.beta.-ketoesters: a selective synthesis of isoflavanones and isoflavones

AUTHOR(S): Donnelly, Dervilla M. X.; Finet, Jean Pierre; Rattigan, Bernard A.

CORPORATE SOURCE: Dep. Chem., Univ. Coll. Dublin, Dublin, Ire.

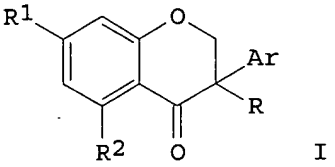
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (15), 1729-35
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

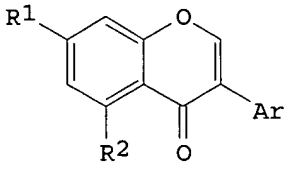
LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:217185

GI



I



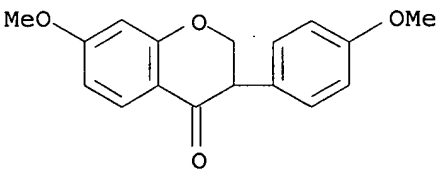
II

AB Arylation of A-ring substituted and unsubstituted 3-allyloxycarbonylchroman-4-ones I (Ar = H, R = CO2CH2CH:CH2, R1 = R2 = H, OMe; Ar = H, R = CO2CH2CH:CH2, R1 = OMe, R2 = H) with aryllead (IV) triacetates followed by selective catalytic deallyloxycarbonylation affords isoflavanones I [Ar = Ph, 4-MeC6H4, 4-MeOC6H4, 2,4-(MeO)2C6H3, 2,4,6-(MeO)3C6H2, R = H] or isoflavones II in high overall yields. The highest yield in the arylation step was obsd. in the reaction of 5,7-dimethoxychroman-4-one with the more hindered 2,4,6-trimethoxyphenyllead triacetate.

IT **15236-11-0P**, 7,4'-Dimethoxyisoflavanone
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 15236-11-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 15 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1993:124232 HCAPLUS

DOCUMENT NUMBER: 118:124232

TITLE: Synthesis and antioxidant activity of isoflavones and isoflavanones

AUTHOR(S): Bulut, Mustafa

CORPORATE SOURCE: Fac. Nat. Sci. Lit., Univ. Marmara, Kadikoy, Turk.

SOURCE: Chimica Acta Turcica (1992), 19(2), 121-8
CODEN: CATUA9; ISSN: 0379-5896

DOCUMENT TYPE: Journal

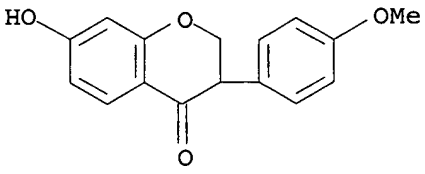
LANGUAGE: German

AB Fifteen hydroxyisoflavones were prepd. and reduced to the hydroxyisoflavanones. Polyhydroxylated isoflavones, particularly 5,7,3',4'-tetrahydroxy- and 6,7-dihydroxyisoflavone, had antioxidant activity, but natural 5,7-dihydroxyisoflavones are not particularly good antioxidants. The isoflavanones were more active than the isoflavones, particularly the 6-hydroxy derivs.

IT **4626-22-6P 17238-05-0P 121927-95-5P**
129159-06-4P 146307-84-8P 146307-85-9P
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. and antioxidant activity of)

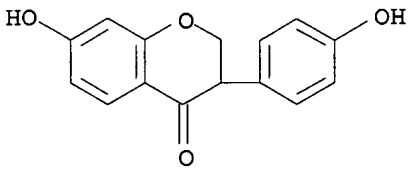
RN 4626-22-6 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



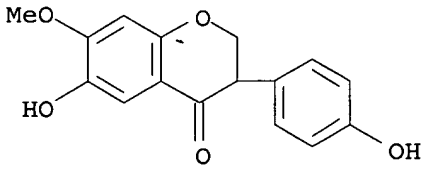
RN 17238-05-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



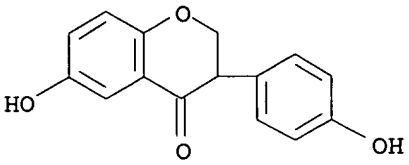
RN 121927-95-5 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6-hydroxy-3-(4-hydroxyphenyl)-7-methoxy- (9CI) (CA INDEX NAME)

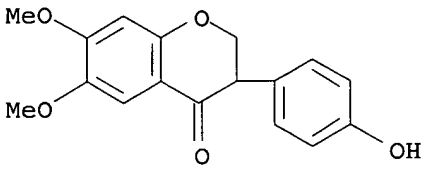


RN 129159-06-4 HCAPLUS

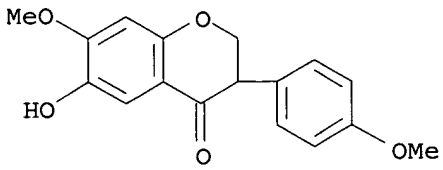
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 146307-84-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-3-(4-hydroxyphenyl)-6,7-dimethoxy- (9CI) (CA INDEX NAME)

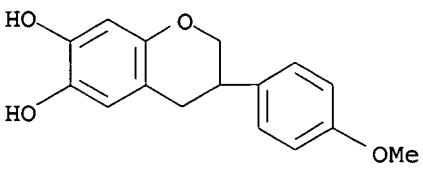


RN 146307-85-9 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6-hydroxy-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

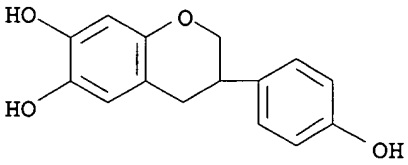


L39 ANSWER 16 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:101686 HCAPLUS
DOCUMENT NUMBER: 118:101686
TITLE: Novel synthesis of isoflavenes and study of the pharmacological properties of their derivatives
AUTHOR(S): Bulut, Mustafa
CORPORATE SOURCE: Natur. Literat. Sci. Fac., Univ. Marmara, Istanbul, Turk.
SOURCE: Chimica Acta Turcica (1992), Volume Date 1991, 19(1), 17-26
CODEN: CATUA9; ISSN: 0379-5896
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Dihydroxydeoxybenzoins, chromones, 3-phenylcoumarins, 3-phenylchromones, and isoflavans were tested for antioxidant activity in vitamin E-free lard. o-Dihydroxy substitution in the arom. ring of the benzopyran moiety led to high antioxidant activity. Some of the compds. were prepd. Thus, 3-phenylchromones were obtained by NaBH4-H3BO3 redn. of isoflavones and by Dibal redn. of 3-phenylcoumarins.
IT **76397-87-0P 94105-89-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. and antioxidant activity of)
RN 76397-87-0 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)- (9CI) (CA

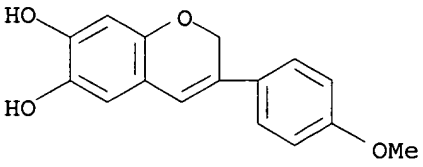
INDEX NAME)



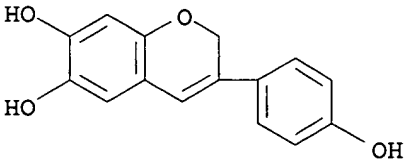
RN 94105-89-2 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IT **145917-92-6P 145917-93-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(prepn., redn., and antioxidant activity of)
RN 145917-92-6 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 145917-93-7 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 17 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:423348 HCAPLUS
DOCUMENT NUMBER: 117:23348
TITLE: Biosynthesis of the A/B/C/D-ring system of the rotenoid amorphigenin by Amorpha fruticosa seedlings
AUTHOR(S): Bhandari, Prabha; Crombie, Leslie; Daniels, Peter; Holden, Ian; Van Bruggen, Nicholas; Whiting, Donald A.

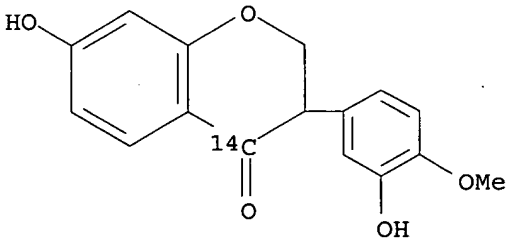
CORPORATE SOURCE: Dep. Chem., Univ. Nottingham, Nottingham, NG7 2RD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1992), (7), 839-49
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB With phenylalanine as a the starting point, the biosynthesis of the characteristic rotenoid A/B/C/D-ring system of amorphigenin is studied using A. fruticosa seedlings. The course of the biosynthesis can be divided into four phases represented by the bordered and interconnecting schemes which summarize the chalcone-flavanone phase, the flavanone-isoflavone phase, the hydroxylation/methoxylation phase and the rotenoid phase. By using an INADEQUATE NMR expt. involving the administration of [1,2-13C]acetate, the type of folding forming ring-D is demonstrated by 13C-13C coupling and is interpreted as involving a polyketide contg. a glutaconate segment which cyclises by a Claisen condensation. The resulting chalcone is cyclized, enzymically and stereospecifically, to 4',7-dihydroxyflavanone. The latter flavanone undergoes aryl migration, in a manner similar to that found in isoflavone biosynthesis, to give 7-hydroxy-4'-methoxyisoflavone. Possible mechanisms for the flavanone-isoflavone rearrangement are discussed, including a proposal that the initiating step involves attack on ring-A and is similar to the first stage of the arom. hydroxylation of tyrosine to dopa. Although possessing no 4'-hydroxy group in ring-A, the mechanism is also applicable to the recently discovered rotenoids of the Boerhaavia and Iris type, and it provides an explanation for the biogenesis of natural spirobenzocyclobutanes from dihydroeucominoids. Six suitably substituted isoflavonoids labeled with 13C or 3H are synthesized and are used to show that the next hydroxylation (and probably methylation) involves C-3' rather than C-2' in 7-hydroxy-4'-methoxyisoflavone. While the methylations involve S-adenosylmethionine, the hydroxylating enzymes are probably very similar to the flavanone-isoflavone-rearranging enzyme. The closure of ring-B to form finally the rotenoid system probably involves conjugate addn. of the methoxyl radical. Prenylation and oxidative modifications are characteristically late-stage processes.

IT **142050-43-9P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

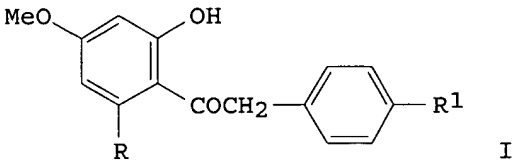
RN 142050-43-9 HCAPLUS

CN 4H-1-Benzopyran-4-one-4-14C, 2,3-dihydro-7-hydroxy-3-(3-hydroxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)

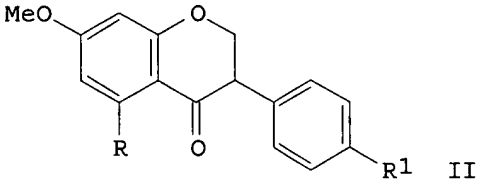


L39 ANSWER 18 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:193973 HCAPLUS
DOCUMENT NUMBER: 116:193973
TITLE: A one-step synthesis of isoflavanones

AUTHOR(S): Hariramakrishnan, K.; Gandhidasan, R.; Raman, P. V.
CORPORATE SOURCE: Sch. Chem., Madurai Kamaraj Univ., Madurai, 625 021, India
SOURCE: Indian Journal of Heterocyclic Chemistry (1991), 1(3), 98
CODEN: IJCHEI; ISSN: 0971-1627
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:193973
GI

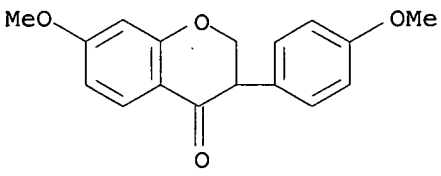


I



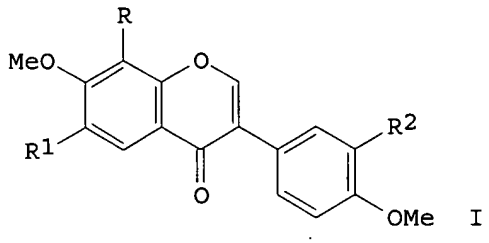
II

AB A simple one step reaction of 2-hydroxydesoxybenzoins I (R, R1 = H, MeO) with (MeO)2CH2 gave isoflavanones II.
IT **15236-11-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

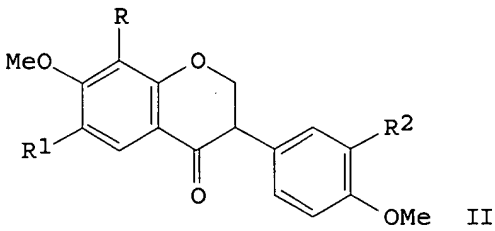


L39 ANSWER 19 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:163807 HCAPLUS
DOCUMENT NUMBER: 114:163807
TITLE: Synthesis of isoflavanones from isoflavones by reduction with sodium hydrogen telluride
AUTHOR(S): Jain, A. C.; Kumar, Ashok; Sharma, Nawal Kishor
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1991), 30B(2), 290-1
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal

LANGUAGE: English
GI



I



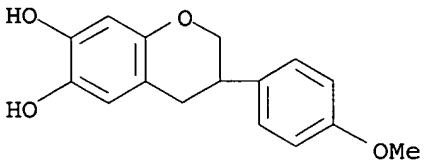
II

AB Redn. of isoflavones I (R = H, OMe, R1 = R2 = H; R = H, R1 = R2 = OMe) with NaHTe gave 61-70.7% isoflavanones II.
IT **67492-32-4P 132974-75-5P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of, by redn. of isoflavone with sodium hydrogen telluride)
RN 67492-32-4 HCAPLUS
RN 132974-75-5 HCAPLUS

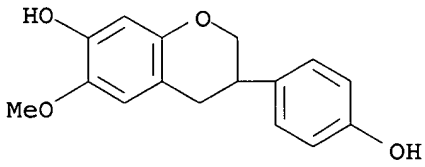
L39 ANSWER 20 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:494654 HCAPLUS
DOCUMENT NUMBER: 113:94654
TITLE: Antifungal activity of isoflavonoids in different reduced stages on Rhizoctonia solani and Sclerotium rolfsii
AUTHOR(S): Weidenboerner, Martin; Hindorf, Holger; Jha, Hem Chandra; Tsotsonos, Prodromos; Egge, Heinz
CORPORATE SOURCE: Inst. Pflanzenkrankheiten, Univ. Bonn, Bonn, D-5300, Germany
SOURCE: Phytochemistry (1990), 29(3), 801-3
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two naturally occurring isoflavones, genistein and iochanin A, and their dihydroderivs. (isoflavanones), as well as 9 perhydrogenated isoflavones (isoflavans), were tested for their effects on mycelial growth of the 2 soil borne fungi Rhizoctonia solani and Sclerotium rolfsii. All the isoflavonoids of the biochanin A series showed high antifungal activity. Genistein isoflavan and the other isoflavans with 2 hydroxyl groups and one methoxy group were fungitoxic, while isoflavan with 2 or 3 methoxy groups were almost inactive.
IT **76397-87-0 94105-91-6 97148-46-4 97148-47-5 128885-09-6 128885-10-9 128885-11-0**

RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antifungal activity of, structure in relation to)

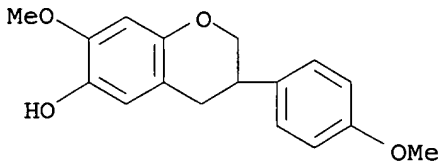
RN 76397-87-0 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



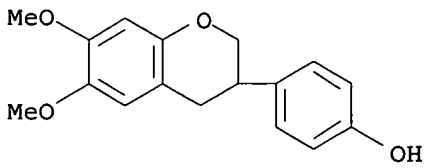
RN 94105-91-6 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(4-hydroxyphenyl)-6-methoxy- (9CI) (CA INDEX NAME)



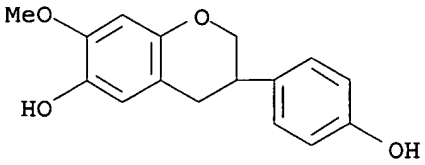
RN 97148-46-4 HCAPLUS
CN 2H-1-Benzopyran-6-ol, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



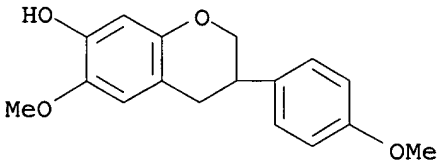
RN 97148-47-5 HCAPLUS
CN Phenol, 4-(3,4-dihydro-6,7-dimethoxy-2H-1-benzopyran-3-yl)- (9CI) (CA INDEX NAME)



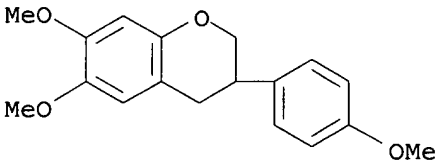
RN 128885-09-6 HCAPLUS
CN 2H-1-Benzopyran-6-ol, 3,4-dihydro-3-(4-hydroxyphenyl)-7-methoxy- (9CI) (CA INDEX NAME)



RN 128885-10-9 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-6-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

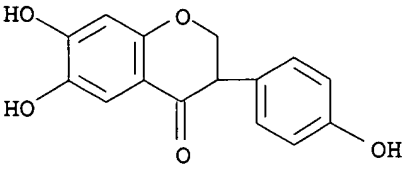


RN 128885-11-0 HCAPLUS
CN 2H-1-Benzopyran, 3,4-dihydro-6,7-dimethoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

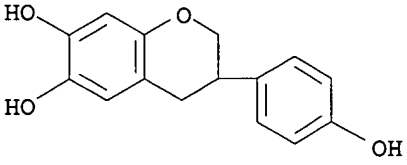


L39 ANSWER 21 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:95337 HCAPLUS
DOCUMENT NUMBER: 112:95337
TITLE: Antifungal activity of isoflavonoids against storage fungi of the genus Aspergillus
AUTHOR(S): Weidenboerner, Martin; Hindorf, Holger; Jha, Hem Chandra; Tsotsonos, Prodromos; Egge, Heinz
CORPORATE SOURCE: Inst. Pflanzenkrankh., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.
SOURCE: Phytochemistry (1989), 28(12), 3317-19
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The fungicidal activity of 2 isoflavones, 1 isoflavanone and 7 isoflavans was tested in malt ext. broth against 5 storage fungi of the genus Aspergillus. While the isoflavones and the isoflavanone show only low activity, the 2 isoflavans 7,8-dihydroxy-4'-methoxyisoflavan and 6,7-dihydroxy-3'-methylisoflavan were highly inhibitory to Aspergillus. Structure-activity relationships are discussed.
IT **94105-87-0 94105-89-2**, 6,7,4'-Trihydroxyisoflavan
94105-90-5 116718-58-2
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antifungal activity of, against Aspergillus)
RN 94105-87-0 HCAPLUS

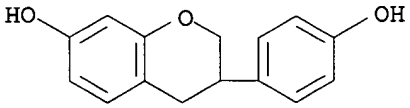
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



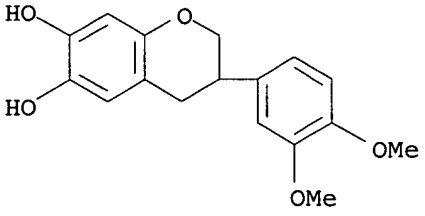
RN 94105-89-2 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 94105-90-5 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

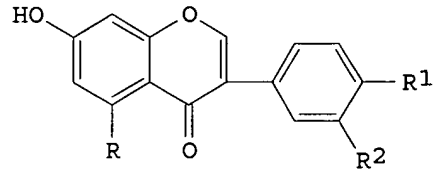


RN 116718-58-2 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3-(3,4-dimethoxyphenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)

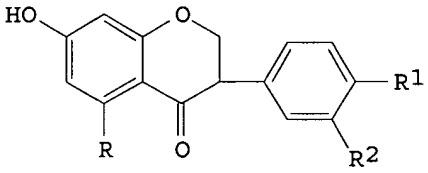


L39 ANSWER 22 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:7203 HCAPLUS
DOCUMENT NUMBER: 112:7203
TITLE: Hydrogen transfer reduction of isoflavones
AUTHOR(S): Wahala, K.; Hase, T. A.
CORPORATE SOURCE: Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SOURCE: Heterocycles (1989), 28(1), 183-6

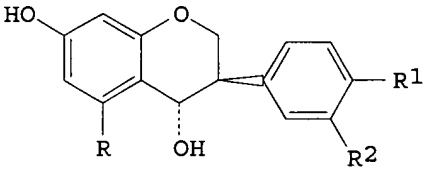
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:7203
GI



I



II

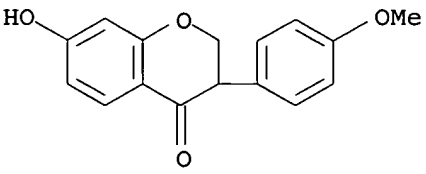


III

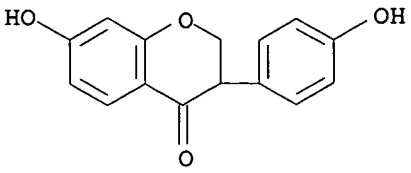
AB H transfer redn. of isoflavones I [R = H, OH; R1 = H, OH, OMe; R2 = H, OMe) using Pd-HCO2NH4 provides easy access to polyoxyisoflavonones II and also to isoflavan-4-ols III without the need for protection of the OH groups. Optimized reaction conditions for improved isoflavonone yields are also discussed.

IT **4626-22-6P 17238-05-0P 124093-18-1P**
124093-19-2P 124093-20-5P 124093-21-6P
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of, by palladium-ammonium formate redn. of isoflavone)

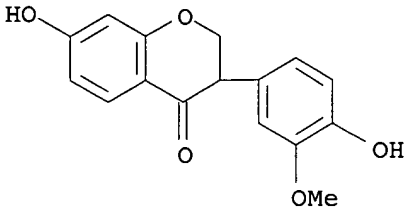
RN 4626-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

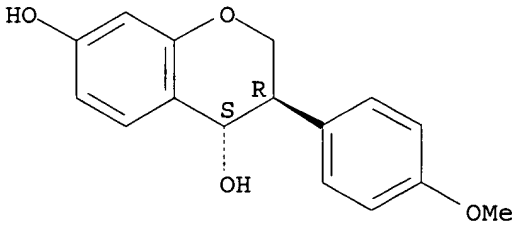


RN 124093-18-1 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-
(9CI) (CA INDEX NAME)



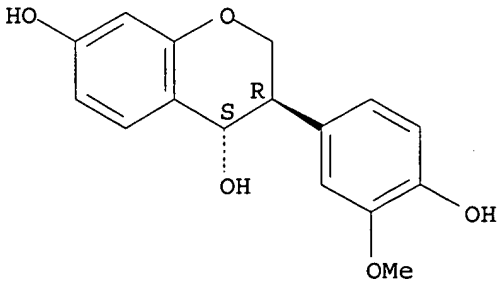
RN 124093-19-2 HCAPLUS
RN 124093-20-5 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-, trans- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



RN 124093-21-6 HCAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-hydroxy-3-methoxyphenyl)-,
trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



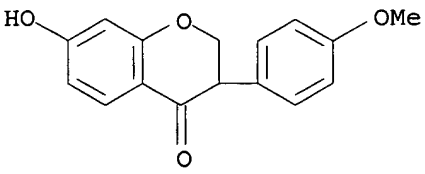
L39 ANSWER 23 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1989:489777 HCAPLUS
DOCUMENT NUMBER: 111:89777
TITLE: Inhibition of cAMP phosphodiesterase in medicinal plants. Part XVI. Inhibition of adenosine 3',5'-cyclic monophosphate phosphodiesterase by flavonoids. III
AUTHOR(S): Nikaido, Tamotsu; Ohmoto, Taichi; Kinoshita, Takeshi; Sankawa, Ushio; Delle Monache, Franco; Botta, Bruno; Tomimori, Tsuyoshi; Miyaichi, Yukinori; Shirataki, Yoshiaki; et al.
CORPORATE SOURCE: Sch. Pharm. Sci., Toho Univ., Funabashi, 274, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1989), 37(5), 1392-5
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English

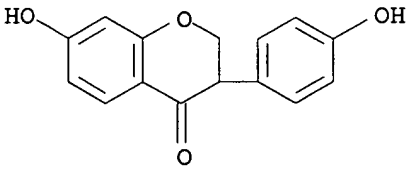
AB Sixty-one flavanones, 26 isoflavones, and 8 other flavonoids, obtained from Sophora tomentosa, S. flavescens, Scutellaria baicalensis and other medicinal plants or synthesized, were tested for their inhibitory activity against cAMP phosphodiesterase from beef heart. Numerous structure-activity relationships are reported.

IT **4626-22-6 17238-05-0 56407-05-7 120185-45-7 120185-46-8 121927-95-5 121927-98-8 121928-00-5**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(cAMP phosphodiesterase inhibition by, structure in relation to)

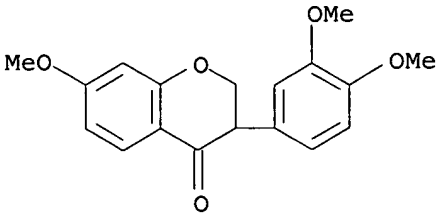
RN 4626-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



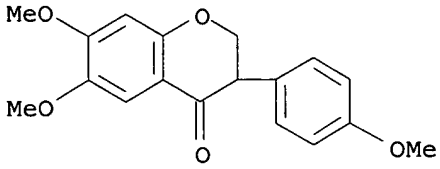
RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



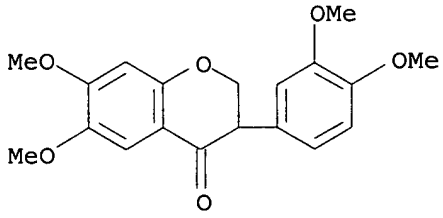
RN 56407-05-7 HCAPLUS
CN 4H-1-Benzopyran-4-one, 3-(3,4-dimethoxyphenyl)-2,3-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



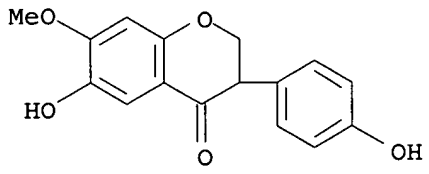
RN 120185-45-7 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6,7-dimethoxy-3-(4-methoxyphenyl)-
(9CI) (CA INDEX NAME)



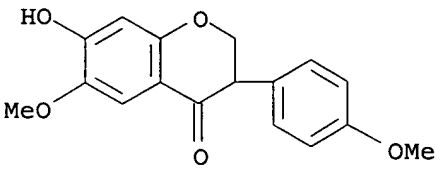
RN 120185-46-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 3-(3,4-dimethoxyphenyl)-2,3-dihydro-6,7-dimethoxy-
(9CI) (CA INDEX NAME)



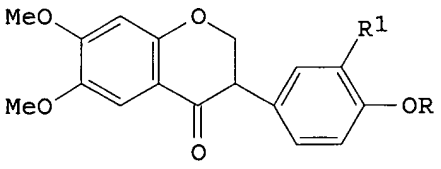
RN 121927-95-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6-hydroxy-3-(4-hydroxyphenyl)-7-methoxy-
(9CI) (CA INDEX NAME)



RN 121927-98-8 HCAPLUS
RN 121928-00-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-6-methoxy-3-(4-methoxyphenyl)-
(9CI) (CA INDEX NAME)



L39 ANSWER 24 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:172924 HCAPLUS
DOCUMENT NUMBER: 110:172924
TITLE: Synthesis of naturally occurring 6,7-dimethoxy-3',4'-methylenedioxyisoflavanone and its analogs
AUTHOR(S): Jain, Amolak C.; Prasad, Ashok K.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1988), 27B(7), 622-4
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:172924
GI

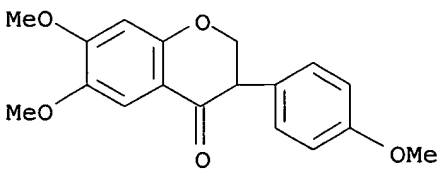


I

AB 6,7-Dimethoxy-3',4'-methylenedioxyisoflavanone (I, RR1 = CH2O), isolated from the heartwood of Cordyla africana, has now been synthesized by the Hoesch condensation of 1,2,4-(HO)3C6H3 with 3,4-methylenedioxybenzyl cyanide; partial methylation, hydroxymethylation, and cyclization. I (R = Me, R1 = H, OMe) have been synthesized similarly.

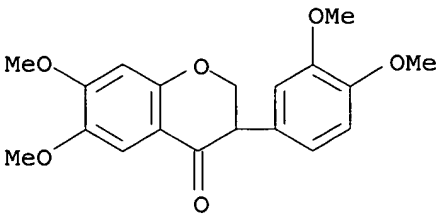
IT **120185-45-7P 120185-46-8P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 120185-45-7 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6,7-dimethoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

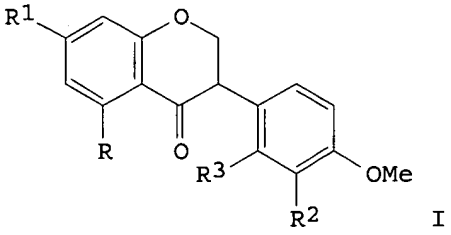


RN 120185-46-8 HCAPLUS

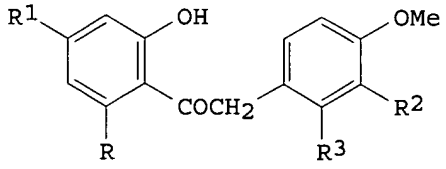
CN 4H-1-Benzopyran-4-one, 3-(3,4-dimethoxyphenyl)-2,3-dihydro-6,7-dimethoxy- (9CI) (CA INDEX NAME)



L39 ANSWER 25 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:23591 HCAPLUS
DOCUMENT NUMBER: 110:23591
TITLE: Synthesis of natural (.+-.)-dihydrocladrin, (.+-.)-homoferreirin, and related isoflavanones
AUTHOR(S): Jain, Amolak C.; Tyagi, Om D.; Prasad, Ashok K.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Proceedings - Indian Academy of Sciences, Chemical Sciences (1988), 100(1), 45-52
CODEN: PIAADM; ISSN: 0253-4134
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:23591
GI



I



II

AB Two naturally occurring isoflavanones, i.e., dihydrocladrin (I; R = R3 = H, R1 = OH, R2 = MeO) and homoferreirin (I; R = R1 = OH, R2 = H, R3 = MeO) and the related compds. di-O-methylhomoferreirin (I; R = R1 = R3 = MeO, R2 = H) and 7-O-methylsativanone (I; R = R2 = H, R1 = R3 = MeO) were prepd. in racemic form from the resp. deoxybenzoins (II; same R-R3) by the EtOCH2Cl method from the literature.

IT **118176-13-9P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

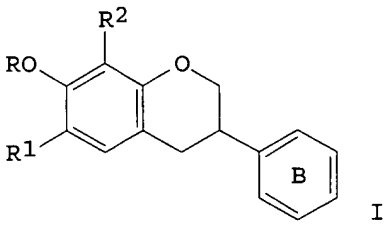
RN 118176-13-9 HCAPLUS

L39 ANSWER 26 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:549354 HCAPLUS
DOCUMENT NUMBER: 109:149354
TITLE: Preparation and formulation of 3-aryl-3,4-dihydro-2H-1-benzopyrans useful in treatment of vascular diseases

INVENTOR(S): Albert, Alban Imre; Zilliken, Friedrich W.
PATENT ASSIGNEE(S): Zyma S. A., Switz.
SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 267155	A2	19880511	EP 1987-810620	19871029
EP 267155	A3	19880720		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
NO 8704489	A	19880505	NO 1987-4489	19871028
FI 8704804	A	19880505	FI 1987-4804	19871102
DD 275048	A5	19900110	DD 1987-308578	19871102
DK 8705756	A	19880505	DK 1987-5756	19871103
ZA 8708245	A	19880629	ZA 1987-8245	19871103
HU 48611	A2	19890628	HU 1987-4930	19871103
AU 8780655	A1	19880505	AU 1987-80655	19871104
AU 606087	B2	19910131		
JP 63130589	A2	19880602	JP 1987-277528	19871104
US 4814346	A	19890321	US 1987-116737	19871104

PRIORITY APPLN. INFO.: GB 1986-26344 19861104
OTHER SOURCE(S): MARPAT 109:149354
GI



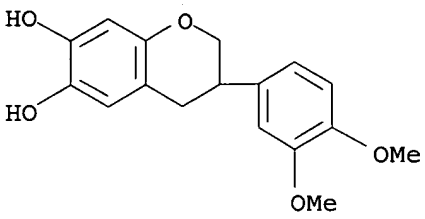
I

AB Title compds. I [R = H, (un)substituted alkyl; one of R1 and R2 = HO, alkoxy, alkanoyloxy, alkyl and the other is H, or ORR1 = (un)substituted OCH2O; R2 = H, or ORR2 = (un)substituted OCH2O; B is (un)substituted by alkyl, phenylalkyl, alkanoyloxy, halo, amino, etc.] and their salts, useful for treatment of vascular diseases (no data) were prepd. 6,7-Dihydroxy-3-(3,4-dimethoxyphenyl)-4H-1-benzopyran-4-one in dioxane and EtOH is hydrogenated for 8 days over Pd/C to give I [R, R2 = H, R1 = HO; B = 3,4-(Me2O)2].

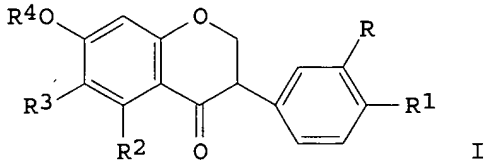
IT **116718-58-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of, for treatment of vascular disease)

RN 116718-58-2 HCAPLUS

CN 2H-1-Benzopyran-6,7-diol, 3-(3,4-dimethoxyphenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)

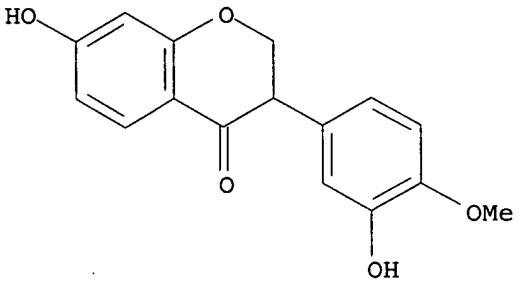


L39 ANSWER 27 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:422691 HCAPLUS
DOCUMENT NUMBER: 109:22691
TITLE: Synthesis of naturally occurring (.+-.)-7,3'-dihydroxy-4'-methoxyisoflavanone and some isoflavanones related to natural 6,7-dimethoxy-3',4'-methylenedioxyisoflavanone
AUTHOR(S): Jain, A. C.; Bambah, P. K.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(7), 628-33
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:22691
GI

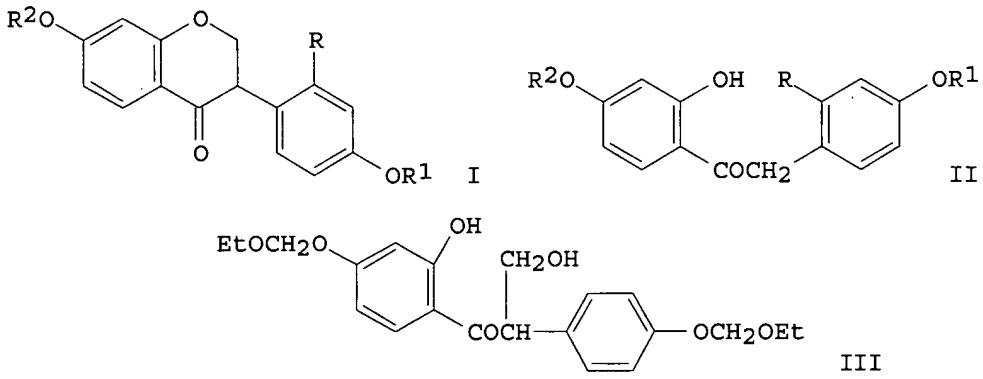


I

AB 2,4,3'-Trihydroxy-4'-methoxydesoxybenzoin on treatment with 2 mol of EtOCH2Cl followed by 1 mol of EtOCH2Cl yields the diether which undergoes cyclization with 4% EtOH-Na2CO3 to afford 7,3'-bis(ethoxymethoxy)-4'-methoxyisoflavanone. Deprotection with 10% MeOH-HCl yields the naturally occurring 7,3'-dihydroxy-4'-methoxyisoflavanone (I, R = OH, R1 = OMe, R2-R4 = H). I (RR1 = OCH2O, R2 = H, OMe, R3 = H, R4 = H, Me; R-R2 = H, R3 = OMe, R4 = Me) were similarly prepd.
IT **67492-31-3P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 67492-31-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(3-hydroxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



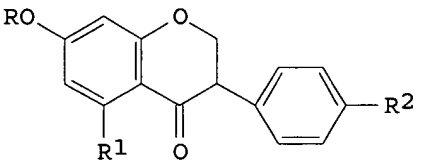
L39 ANSWER 28 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:131344 HCAPLUS
DOCUMENT NUMBER: 108:131344
TITLE: Synthesis of (.+-.)-sativanone and (.+-.)-dihydrodaidzein
AUTHOR(S): Jain, Amolak C.; Nayyar, Naresh K.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(2), 136-9
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:131344
GI



AB The title compds. (I; R = MeO, R1 = Me, R2 = H; R-R2 = H) resp. were prepd in 3 steps from desoxybenzoins II. Thus, II (R-R2 = H) was treated with 3 equiv of EtOCH2Cl to give 87% hydroxydesoxybenzoin III which was cyclized with Na2CO3 to give 70% I (R = H, R1 = R2 = EtOCH2). Deprotection with HCl-MeOH gave 91% I (R-R2 = H).
IT **37054-07-2P**, (.+-.)-Dihydrodaidzein
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(total synthesis of)
RN 37054-07-2 HCAPLUS

L39 ANSWER 29 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:552767 HCAPLUS
DOCUMENT NUMBER: 105:152767

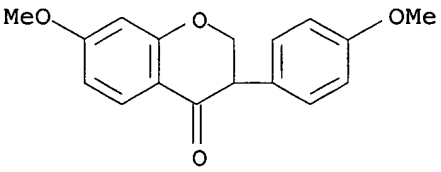
TITLE: A new general synthesis of hydroxy- and methoxyisoflavanones
AUTHOR(S): Jain, Amolak C.; Mehta, Anita
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1986), (2), 215-20
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:152767
GI



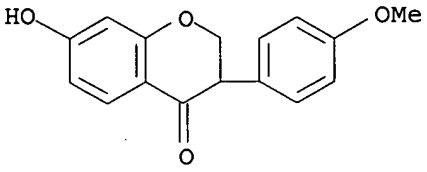
I

AB A new general synthesis of isoflavanones I (R = H, Me, CH2OEt; R1 = H1OH, OMe, OCH2OEt; R2 = H, OMe) has been accomplished in overall yields of 47-73% from 2,4,6-R1(RO)(HO)C6H2COCH2C6H4R2-4. The first step involves with EtOCH2Cl in the presence of dry K2CO3 which gives 2,4,6-R1(RO)(HO)C6H2COCH(CH2OH)C6H4R2-4 (II). The explanation for the unexpected formation has been provided on the basis of an elimination-addn. mechanism. Subsequent refluxing with Na2CO3 in aq EtOH afforded I (R = Me, CH2OEt; R1 = H, OMe, OCH2OEt). Final removal of the ethoxymethyl groups with 10% MeOH-HCl afforded I (R = H, R1-OH).

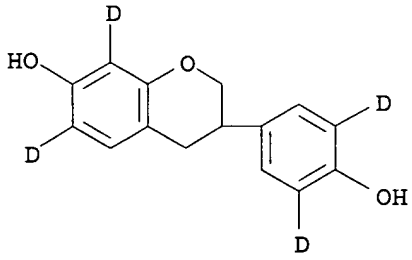
IT **15236-11-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of)
RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **4626-22-6P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. and ether cleavage of)
RN 4626-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

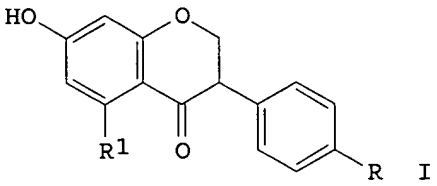


L39 ANSWER 30 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:533626 HCAPLUS
DOCUMENT NUMBER: 105:133626
TITLE: Synthesis of the [2H]-labeled urinary lignans, enterolactone and enterodiol, and the phytoestrogen daidzein and its metabolites equol and O-demethylangolensin
AUTHOR(S): Wahala, Kristiina; Makela, Taru; Backstrom, Reijo; Brunow, Gosta; Hase, Tapio
CORPORATE SOURCE: Dep. Chem., Univ. Helsinki, Helsinki, 00100, Finland
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1986), (1), 95-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:133626
AB [2H6]enterolactone, [2H6]enterodiol, [2H4]daidzein, [2H4]equol, [2H5]-O-demethylangolensin, were prepd. by D exchange using PBr3 or NaOD in DO or CF3CO2D.
IT **104411-14-5P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 104411-14-5 HCAPLUS
CN 2H-1-Benzopyran-6,8-d2-7-ol, 3,4-dihydro-3-(4-hydroxyphenyl-3,5-d2)- (9CI) (CA INDEX NAME)



L39 ANSWER 31 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:487683 HCAPLUS
DOCUMENT NUMBER: 103:87683
TITLE: A new general synthesis of polyhydroxyisoflavanones
AUTHOR(S): Jain, Amolak C.; Sharma, Anita
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Journal of the Chemical Society, Chemical Communications (1985), (6), 338-9
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:87683
GI



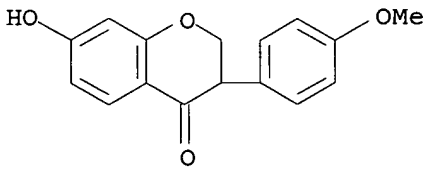
I

AB Hydroxyisoflavanones were prepd. in 4 steps from polyhydroxydeoxybenzoins in 45-57% overall yield. E.g., sequential treatment of 2,4,6-(HO)3C6H2COCH2Ph with ClCH2OEt and dry K2CO3 in Me2CO at room temp., ClCH2OEt at 60-70.degree. for 1-1.5 h, 4% aq. ethanolic Na2CO3 for 2-3 h, and 10% methanolic HCl for 7-10 min gave hydroxyisoflavanone I (R = H, R1 = OH) in 57.0% overall yield. I (R = H, OMe; R1 = H) were similarly prepd.

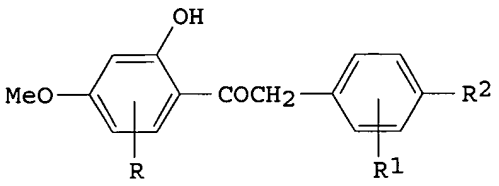
IT **4626-22-6P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 4626-22-6 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 32 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:406088 HCAPLUS
DOCUMENT NUMBER: 103:6088
TITLE: Hydroxymethylation studies of o-hydroxyphenyl benzyl ketones with and without the use of phase transfer catalyst: a novel synthesis of isoflavanones
AUTHOR(S): Jain, P. K.; Pinkey; Makrandi, J. K.; Grover, S. K.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1985), 24B(1), 51-8
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:6088
GI



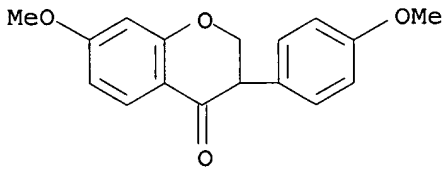
I

AB o-Hydroxyphenyl ketones I (R = H, 3-Me, 5-Me; R1 = H, 2-OMe, 3-OMe; R2 = H, OMe) on treatment with CH2O in a CHCl3-aq. K2CO3 biphase system, give the corresponding .alpha.-hydroxymethyl derivs. This reaction, when carried out in the presence of a phase-transfer catalyst, leads to 3-hydroxymethylisoflavanones. I (R = 6-OMe, R1 = H, R2 = H, OMe) also give the .alpha.-hydroxymethyl derivs. under phase-transfer catalyzed conditions. However, in the absence of the phase-transfer catalyst, the reaction product is a complex mixt. The .alpha.-hydroxymethyl-o-hydroxyphenyl benzyl ketones, on refluxing with Et2NH-EtOH afford the corresponding isoflavanones quant. The 3-hydroxymethylisoflavanones, on treatment with K2CO3-H2O-MeOH at 40.degree. undergo dehydroxymethylation to isoflavanones.

IT **15236-11-0P 56407-05-7P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

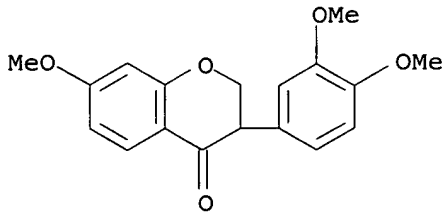
RN 15236-11-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 56407-05-7 HCAPLUS

CN 4H-1-Benzopyran-4-one, 3-(3,4-dimethoxyphenyl)-2,3-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



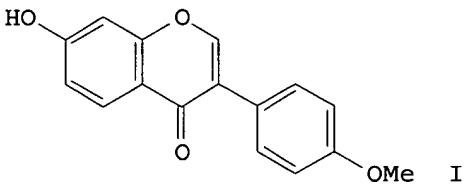
L39 ANSWER 33 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1985:128914 HCAPLUS

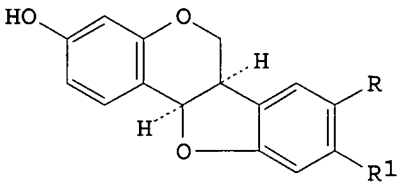
DOCUMENT NUMBER: 102:128914

TITLE: Isoflavonoid biosynthesis: concerning the aryl migration

AUTHOR(S): Al-Ani, Hakim A. M.; Dewick, Paul M.
CORPORATE SOURCE: Dep. Pharm., Univ. Nottingham, Nottingham, NG7 2RD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (12), 2831-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

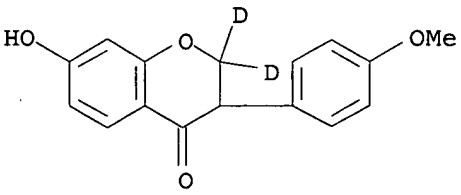


I



II

AB Feeding expts. with 13C- or D-labeled precursors in CuCl2-treated Irifolium pratense seedlings showed that formononetin (I), medicarpin (II; R = H, R1 = OMe) (III), and maackiain (II; RR1 = OCH2O) (IV) are formed from 2',4,4'-trihydroxychalcone by a rearrangement involving an intramol. migration of the cinnamate-derived arom. ring. In all 3 compds., this is accompanied by retention of the chalcone .beta.-H and loss of the .alpha.-H. During formation of IV from I, an NIH shift of D resulting from arom. hydroxylation ortho to the OMe group was obsd. Expts. with 7-hydroxy-4'-methoxyisoflavanone-2-d2 showed that this compd. may be converted into III without loss of D, thus confirming the existence of a metabolic grid of isoflavones and isoflavanones. The results are explained in terms of an oxidative process in which a chalcone is converted into an isoflavone as the 1st-formed isoflavonoid deriv.
IT **95307-73-6P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 95307-73-6 HCAPLUS
CN 4H-1-Benzopyran-4-one-2-d, 2,3-dihydro-2-d-7-hydroxy-3-(4-methoxyphenyl)-(9CI) (CA INDEX NAME)



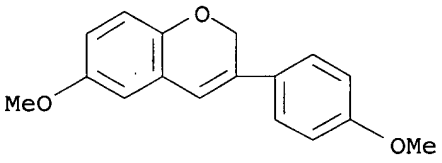
L39 ANSWER 34 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:113112 HCAPLUS
DOCUMENT NUMBER: 102:113112
TITLE: A synthesis of 2,4-dihydroxyisoflavans and 2-hydroxyisoflav-3-enes: versatile precursors to isoflavanoids

AUTHOR(S): Liepa, Andris J.
CORPORATE SOURCE: Div. Appl. Org. Chem., CSIRO, Melbourne, 3001, Australia
SOURCE: Australian Journal of Chemistry (1984), 37(12), 2545-58
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:113112

AB A new synthesis of isoflavanoids was developed by treatment of a salicylaldehyde with an arylglycidate salt. Reaction conditions were found so that this condensation yields either a 2,4-dihydroxyisoflavan or a 2-hydroxyisoflav-3-ene. The 2-hydroxyisoflav-3-ene can then be converted into the isoflavylium salt, isoflavan, 2-hydroxyisofalvan, isoflav-2-ene or isoflav-3-ene. Similarly, the 2-aminoisoflav-3-ene deriv. can be obtained. The reaction of isoflavylium salts with HSCH2CH2CO2H gives carboxyethylthioisoflav-3-ene derivs. potentially useful as haptens for conjugation with suitable macromols. for the generation of antibodies.

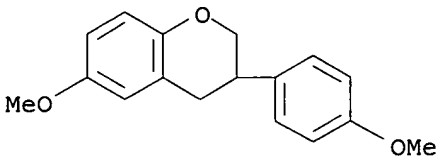
IT **95332-12-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenation of)

RN 95332-12-0 HCAPLUS
CN 2H-1-Benzopyran, 6-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



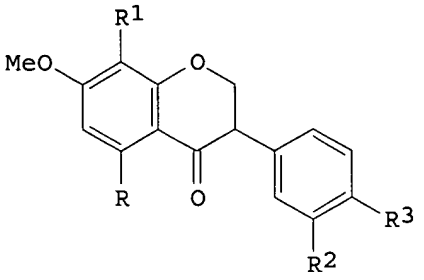
IT **95332-13-1P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 95332-13-1 HCAPLUS
CN 2H-1-Benzopyran, 3,4-dihydro-6-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 35 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:45739 HCAPLUS
DOCUMENT NUMBER: 102:45739
TITLE: Synthesis of methoxyisoflavanones from arylmethyl o-hydroxyaryl ketones and paraformaldehyde
AUTHOR(S): Pinkey; Jain, Pramod K.; Grover, Surinder K.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110007, India
SOURCE: Gazzetta Chimica Italiana (1984), 114(7-8), 355-7

CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

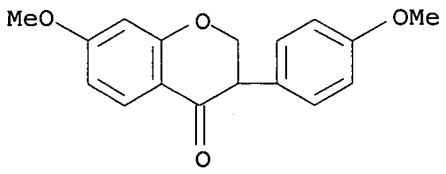


I

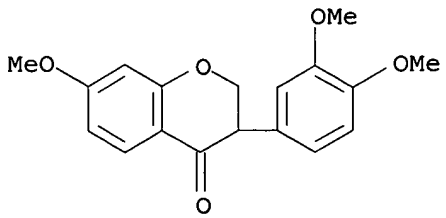
AB The cyclocondensation of 2-hydroxy-4-methoxyphenyl benzyl ketones with HCHO gave isoflavanones I (R = H, OMe; R1 = Me, H; R2 = H OMe; R3 = H, OMe). Thus, benzyl 2-hydroxy-3-methyl-4-methoxyphenyl ketone was heated with HCHO and Et2NH in MeOH to give I (R1 = Me, R = R2 = R3 = H).

IT **15236-11-0P 56407-05-7P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 56407-05-7 HCAPLUS
CN 4H-1-Benzopyran-4-one, 3-(3,4-dimethoxyphenyl)-2,3-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



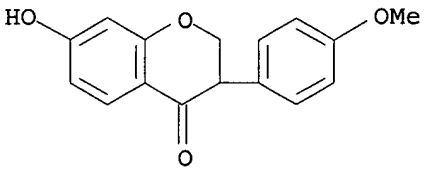
L39 ANSWER 36 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:42728 HCAPLUS
DOCUMENT NUMBER: 102:42728

TITLE: Antifungal activity of soybean and chickpea isoflavones and their reduced derivatives
AUTHOR(S): Kraemer, Rainer Philipp; Hindorf, Holger; Jha, Hem Chandra; Kallage, Jutta; Zilliken, Fritz
CORPORATE SOURCE: Inst. Pflanzenkrankh., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.
SOURCE: Phytochemistry (Elsevier) (1984), 23(10), 2203-5
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English

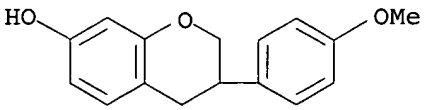
AB The fungicidal activity of the isoflavones from soybean (Glycine max) and chickpea (Cicer arietinum) was studied on 3 food- and forage-contaminating fungi, Aspergillus ochraceus, Penicillium digitatum, and Fusarium culmorum. The reduced derivs. of the corresponding isoflavones, the isoflavanones and isoflavans, were also included in the investigation. For the 1st time in a comparative study it was shown that isoflavones and isoflavanones are variable in their activity whereas the isoflavans are moderately active inhibitors of fungal growth.

IT **4626-22-6 10499-17-9 17238-05-0**
94105-87-0 94105-88-1 94105-89-2
94105-90-5 94105-91-6
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antifungal activity of)

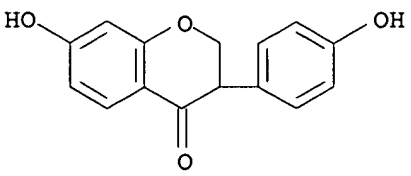
RN 4626-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



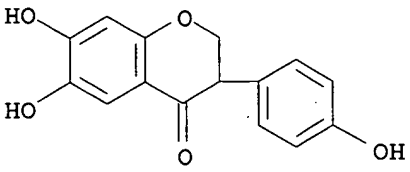
RN 10499-17-9 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



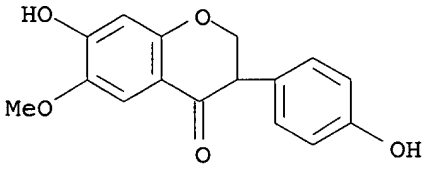
RN 17238-05-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



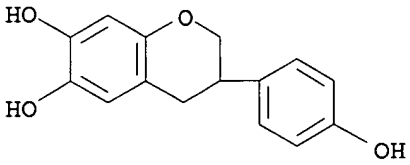
RN 94105-87-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6,7-dihydroxy-3-(4-hydroxyphenyl)-(9CI) (CA INDEX NAME)



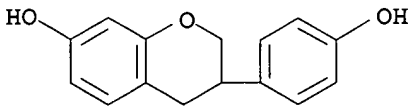
RN 94105-88-1 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-hydroxyphenyl)-6-methoxy-(9CI) (CA INDEX NAME)



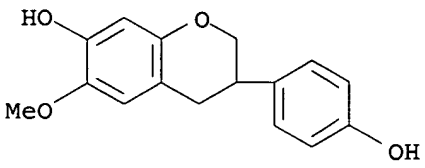
RN 94105-89-2 HCAPLUS
CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



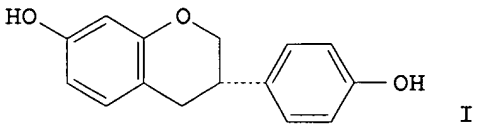
RN 94105-90-5 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 94105-91-6 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(4-hydroxyphenyl)-6-methoxy- (9CI) (CA INDEX NAME)



L39 ANSWER 37 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:19261 HCAPLUS
DOCUMENT NUMBER: 102:19261
TITLE: Characterization of the estrogenic properties of a nonsteroidal estrogen, equol, extracted from urine of pregnant macaques
AUTHOR(S): Thompson, M. A.; Lasley, B. L.; Rideout, B. A.; Kasman, L. H.
CORPORATE SOURCE: Res. Dep., San Diego Zoo, San Diego, CA, USA
SOURCE: Biology of Reproduction (1984), 31(4), 705-13
CODEN: BIREBV; ISSN: 0006-3363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

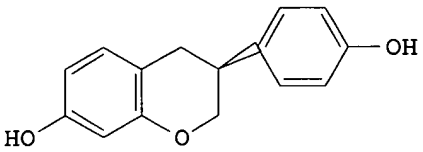


I

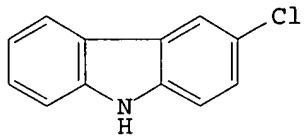
AB The estrogenic activity of equol (I) [531-95-3] from macaque urine, (.+-.)-I [66036-38-2], and 17.beta.-estradiol (E2) [50-28-2] was compared in vitro and in vivo. Relative binding affinity of I for rat uterine receptor was 1% that of E2, and the dissocn. rate of I from the receptor was very high. I was ineffective in stimulating rat uterine wt. gain and possessed limited ability to increase progesterone [57-83-0] receptor. Uterine nuclear receptors, after doses of I sufficient to produce depletion and replenishment of cytosol estrogen receptor, were not measurable by exchange assay. No antiestrogenic activity of I could be demonstrated. The weak potency and lack of antiestrogenic activity of I are difficult to reconcile with its ability to induce ovine infertility. Species differences at some level other than classical estrogen receptor as defined in the rat model may be responsible for variability in the impact of I.
IT **66036-38-2**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(estrogenic activity of)
RN 66036-38-2 HCAPLUS

L39 ANSWER 38 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:96557 HCAPLUS
DOCUMENT NUMBER: 100:96557
TITLE: Isolation and identification of "diazepam-like"

compounds from bovine urine
AUTHOR(S): Luk, Kin Chun; Stern, Lorraine; Weigele, Manfred; O'Brien, Robert A.; Spirt, Nena
CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-LaRoche, Inc., Nutley, NJ, USA
SOURCE: Journal of Natural Products (1983), 46(6), 852-61
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



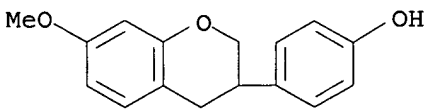
I



II

AB Putative endogenous ligands for the benzodiazepine receptor were isolated from bovine urine. These included 3 isoflavans which had activity like that of diazepam [439-14-5] in a receptor-binding assay: equol (I) [531-95-3], dl-3',7-dihydroxyisoflavan [89019-82-9], and dl-4'-hydroxy-7-methoxyisoflavan [89019-86-3]. Another compd., 3-chloro-9H-carbazole (II) [2732-25-4], enhanced the binding of diazepam in the receptor assay. Pinosylvin monomethyl ether [35302-70-6], indigo [482-89-3], and indirubin [479-41-4] were isolated as inactive compds. Prepns. for many of the compds. isolated are described.

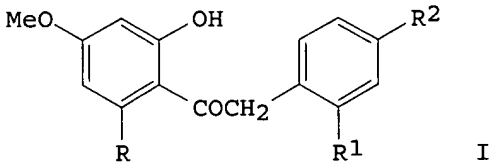
IT **89019-86-3P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. and isolation of, from urine, diazepam-mimetic activity in relation to)
RN 89019-86-3 HCAPLUS
CN Phenol, 4-(3,4-dihydro-7-methoxy-2H-1-benzopyran-3-yl)- (9CI) (CA INDEX NAME)



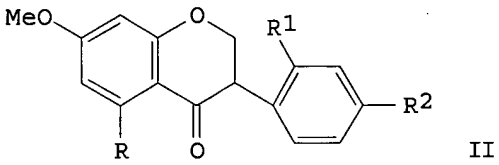
IT **89064-53-9P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 89064-53-9 HCAPLUS

L39 ANSWER 39 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:89120 HCAPLUS
DOCUMENT NUMBER: 98:89120
TITLE: A convenient phase transfer catalyzed synthesis of isoflavanones
AUTHOR(S): Singh, Harcharan; Jain, P. K.; Makrandi, J. K.; Grover, S. K.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1982), 21B(6), 547-8

CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



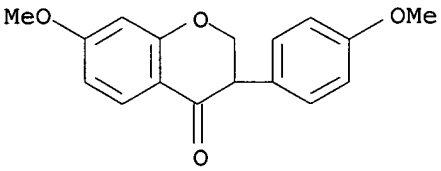
I



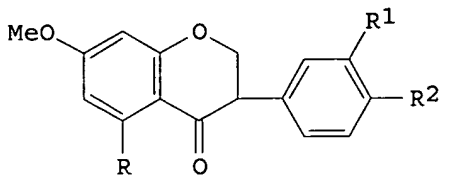
II

AB o-Hydroxyphenyl benzyl ketones I (R-R2 = H, OMe) on treatment with CH2I2 under phase transfer catalyzed conditions in the presence of Bu4N+I- and Na2S2O3 undergo smooth conversion into the isoflavanones II in 60-70% yields.

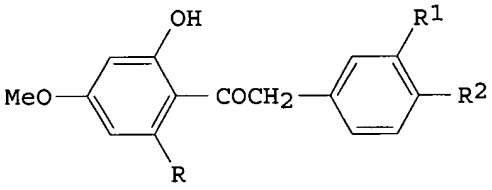
IT **15236-11-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 40 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:89018 HCAPLUS
DOCUMENT NUMBER: 98:89018
TITLE: A new one-pot synthesis of isoflavanones
AUTHOR(S): Gandhidasan, R.; Neelakantan, S.; Raman, P. V.
CORPORATE SOURCE: Dep. Nat. Prod. Chem., Madurai Kamaraj Univ., Madurai, 625 021, India
SOURCE: Synthesis (1982), (12), 1110
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



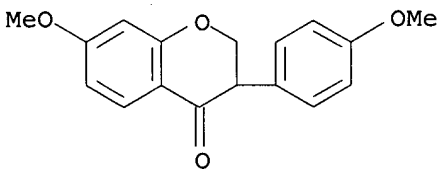
II

AB Isoflavanones I (R, R1 = H, OMe, R2 = H; R1R2 = OCH2O) were obtained in 51-67% yield by cyclizing the hydroxy ketones II with CH2O in the presence of NHMe2.

IT **15236-11-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 15236-11-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 41 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1982:142516 HCAPLUS

DOCUMENT NUMBER: 96:142516

TITLE: A synthesis of hydroxylated isoflavylium salts and their reduction products

AUTHOR(S): Liepa, Andris J.

CORPORATE SOURCE: Div. Appl. Org. Chem., CSIRO, Melbourne, 3001, Australia

SOURCE: Australian Journal of Chemistry (1981), 34(12), 2647-55
CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal

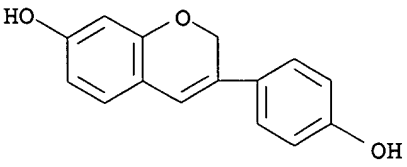
LANGUAGE: English

AB Phloroglucinol reacts with arylmalondialdehydes in the presence of HCl to form 5,7-dihydroxyisoflavylium salts. Redn. of these salts can be utilized to form isoflav-2-enes, isoflav-3-enes or isoflavans.

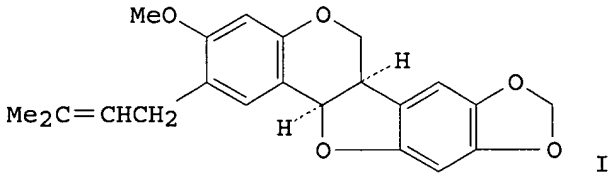
IT **81267-65-4P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 81267-65-4 HCAPLUS

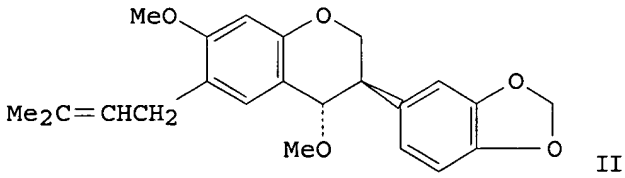
CN 2H-1-Benzopyran-7-ol, 3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



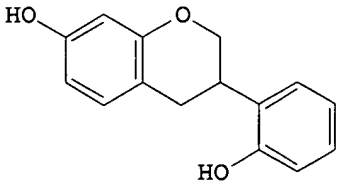
L39 ANSWER 42 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:603790 HCAPLUS
DOCUMENT NUMBER: 95:203790
TITLE: Some photochemical and oxidative conversions of pterocarpans and isoflavans: functional requirements for cyclization of isoflavans to pterocarpans
AUTHOR(S): Breytenbach, Jaco C.; Van Zyl, Jan J.; Van der Merwe, Pieter J.; Rall, Gerhardus J. H.; Roux, David G.
CORPORATE SOURCE: Dep. Chem., Univ. Orange Free State, Bloemfontein, 9300, S. Afr.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1981), (10), 2684-91
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



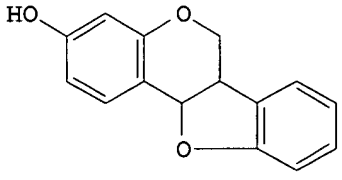
I



II



III

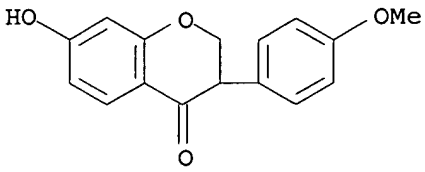


IV

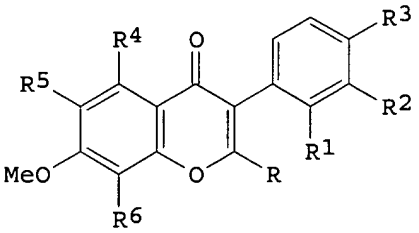
AB Photolysis of pterocarpans in MeOH or AcOH gave 4-functionalized 2'-hydroxy-3,4-trans-isoflavan by C-ring fission and solvolysis. E.g., irradn. of I (MeOH, 300 nm) gave the benzopyran deriv. II (22%). In some cases, spontaneous recyclization to the pterocarpan occurred; this was governed by functional dependent factors such as the effective delocalization of the transient 4-carbocation and formation of quinone

methide intermediates. The oxidative cyclization of 2,7'-dihydroxyisoflavans to pterocarpans by DDQ was also studied. E.g., treatment of III with DDQ (C6H6, under N2, room temp., 15 min) gave IV (65%). This reaction proceeds via unstable quinone methides, or via 4-carbocations after H- abstraction.

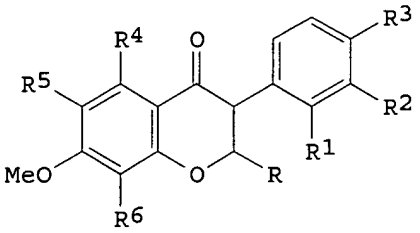
IT **4626-22-6P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 4626-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 43 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:587004 HCAPLUS
DOCUMENT NUMBER: 95:187004
TITLE: Unusual regioselectivity in the reduction of .alpha.,.beta.-unsaturated carbonyl compounds with diisobutylaluminum hydride (DIBAH): direct conversion of isoflavones to isoflavan-4-ones
AUTHOR(S): Antus, Sandor; Gottsegen, Agnes; Nogradi, Mihaly
CORPORATE SOURCE: Res. Group Alkaloid Chem., Hung. Acad. Sci., Budapest, 1521, Hung.
SOURCE: Synthesis (1981), (7), 574-6
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB Isoflavones I (R = H, Me; R1 = OCH2Ph, H; R2 = OMe, H; R3 = OMe, H; R4 = H, OMe; R5 = H, OMe; R6 = H, Me) were converted to the resp. isoflavanones II. A soln. of (Me2CHCH2)2AlH in PhMe was added to I (R = R1 = R2 = R3 = R4 = R5 = R6 = H) in PhMe and THF under Ar at -65.degree., and the mixt. was quenched with MeOH, allowed to warm to room temp., and worked up to give II (R = R1 = R2 = R3 = R4 = R5 = R6 = H).

IT **67492-32-4P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)

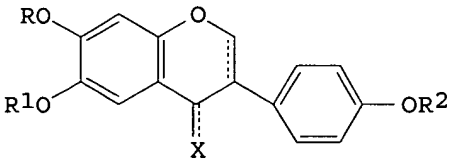
(prepn. of)
RN 67492-32-4 HCAPLUS

L39 ANSWER 44 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:513769 HCAPLUS
DOCUMENT NUMBER: 95:113769
TITLE: Isoflavones and related compounds and antioxidant compositions containing them
INVENTOR(S): Zilliken, Fritz W.
PATENT ASSIGNEE(S): Z-L Ltd. Partnership, USA
SOURCE: U.S., 9 pp. Cont.-in-part of U.S. 4,157,984.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4264509	A	19810428	US 1979-29122	19790411
US 4157984	A	19790612	US 1977-804594	19770608
CA 1140560	A1	19830201	CA 1979-327756	19790516
WO 8002098	A1	19801016	WO 1979-US347	19790518
W: BR, DK, JP				
RW: AT, CH, DE, FR, GB, LU, SE				
BR 7909002	A	19810331	BR 1979-9002	19790518
JP 56500493	T2	19810416	JP 1979-501868	19790518
EP 27796	A1	19810506	EP 1979-901460	19790518
EP 27796	B1	19840711		
R: AT, CH, DE, FR, GB, LU, SE				
AT 8324	E	19840715	AT 1979-901460	19790518
NL 7906193	A	19801014	NL 1979-6193	19790814
DK 8005288	A	19801211	DK 1980-5288	19801211
US 4366082	A	19821228	US 1981-223941	19810112
US 4390559	A	19830628	US 1981-223942	19810112
US 4366248	A	19821228	US 1981-226509	19810119

PRIORITY APPLN. INFO.:
US 1977-804594 19770608
US 1979-29122 19790411
EP 1979-901460 19790518
WO 1979-US347 19790518

GI



I

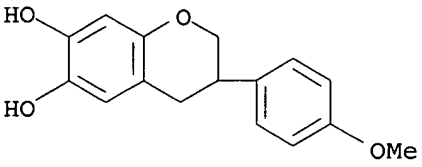
AB Isoflavones and related compds. with the general structure (I; where R, R1, and R2 = H or Me or Et, X = 2H or O, and dashed lines are single or double bonds) are synthesized or purified from Rhizopus-fermented soybeans (tempeh) and optionally modified. These compds. have antioxidant activity in fats and oils. Thus, 6 g texasin (6,7-dihydroxy-3-(4-methoxyphenol)chromone) [897-46-1] was dissolved and partially suspended in 500 mL EtOH and hydrogenated until no starting material was detectable with a Pd on charcoal catalyst with Et3N addn. The hydrogenation catalyst

was removed by filtration, water added, and the EtOH of the reaction mixt. was removed by evapn. at reduced pressure. The ppt. formed during evapn. was identified as 6,7-dihydroxy-3-(4-methoxyphenyl)-chromanon-4 [76397-85-8], which had good antioxidant activity as assessed by the Swift stability test on lard.

IT **76397-87-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. and antioxidant properties of)

RN 76397-87-0 HCAPLUS

CN 2H-1-Benzopyran-6,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

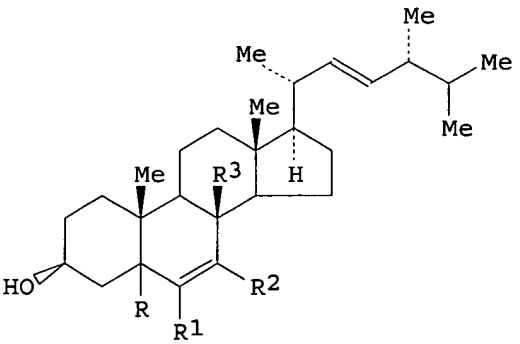


L39 ANSWER 45 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:96313 HCAPLUS
DOCUMENT NUMBER: 94:96313
TITLE: Ergostadienetriols
PATENT ASSIGNEE(S): Z-L Ltd., USA
SOURCE: Neth. Appl., 16 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 7906287	A	19800923	NL 1979-6287	19790817
US 4234577	A	19801118	US 1979-22202	19790319

PRIORITY APPLN. INFO.: US 1979-22202 19790319
US 1977-804594 19770608

GI



I, R=R3=OH, R1=R2=H
II, R=R3=H, R1=R2=OH

AB Ergostadienetriols are useful as hypocholesteremics and as antioxidants for foods. For example, chickens on a diet high in cholesterol and given

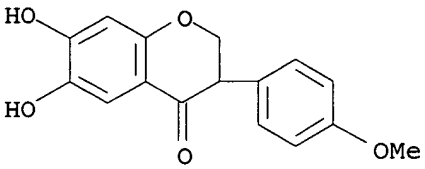
0.1% I [76420-88-7] in the feed had a serum cholesterol level of 283.8 mg%, compared to 330.7 mg% in similar chickens not given I; I was 10-fold more effective than .beta.-sitosterol. Addn. of II [71420-27-4] (0.1% by wt.) to lard provided 50% inhibition of oxidn. by air at 60.degree. over a period of 72 h.

IT **76397-86-9 76420-89-8**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antioxidant activity of)

RN 76397-86-9 HCAPLUS
CN Ergosta-6,22-diene-3,6,7-triol, (3.beta.,22E)-, mixt. with 2,3-dihydro-6,7-dihydroxy-3-(4-methoxyphenyl)-4H-1-benzopyran-4-one (9CI) (CA INDEX NAME)

CM 1

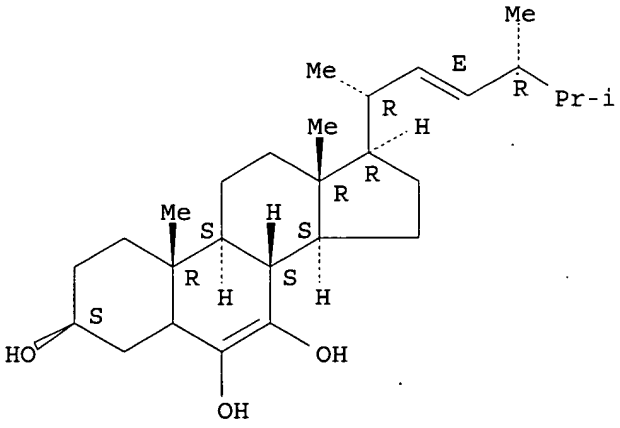
CRN 76397-85-8
CMF C16 H14 O5



CM 2

CRN 71420-27-4
CMF C28 H46 O3

Absolute stereochemistry.
Double bond geometry as shown.

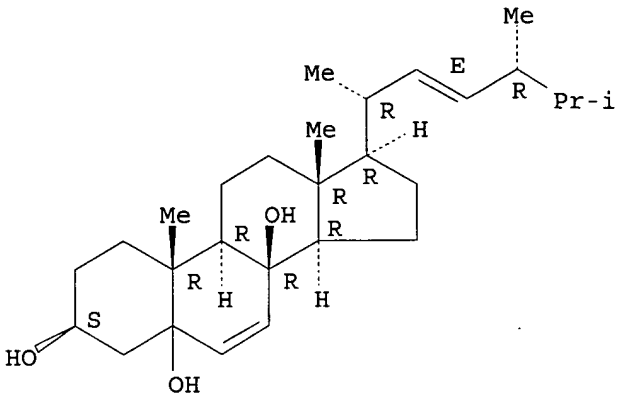


RN 76420-89-8 HCAPLUS
CN Ergosta-6,22-diene-3,5,8-triol, (3.beta.,22E)-, mixt. with 3,4-dihydro-3-(4-methoxyphenyl)-2H-1-benzopyran-6,7-diol (9CI) (CA INDEX NAME)

CM 1

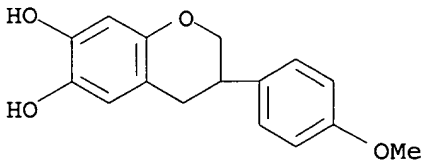
CRN 76420-88-7
CMF C28 H46 O3

Absolute stereochemistry.
Double bond geometry as shown.

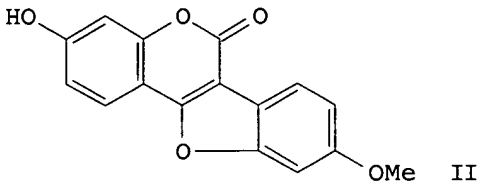


CM 2

CRN 76397-87-0
CMF C16 H16 O4



L39 ANSWER 46 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1979:589838 HCAPLUS
DOCUMENT NUMBER: 91:189838
TITLE: Biosynthesis of pterocarpan, isoflavan and coumestan metabolites of Medicago sativa: chalcone, isoflavone and isoflavanone precursors
AUTHOR(S): Dewick, Paul M.; Martin, Maria
CORPORATE SOURCE: Dep. Pharm., Univ. Nottingham, Nottingham, UK
SOURCE: Phytochemistry (Elsevier) (1979), 18(4), 597-602
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



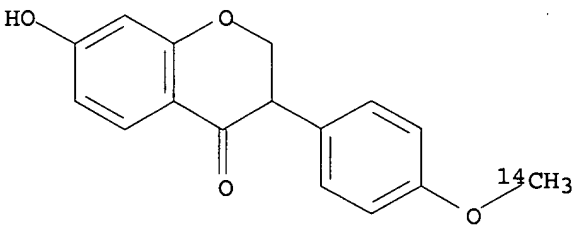
II

AB Feeding expts. on CuCl2- and UV-treated lucerne seedlings indicated that 14C-labeled 2',4,4'-trihydroxychalcone and formononetin but not 2',4'-dihydroxy-4-methylchalcone or daidzein were incorporated into demethylhomopterocarpan (I), sativan, vestitol, and 9-O-methylcoumestrol (II). II formation was stimulated under these conditions but coumestrol prodn. was unaffected. Daidzein and the trihydroxychalcone were precursors of coumestrol. A mechanism is proposed in which methylation is an integral part of the aryl migration process assocd. with the formation of 4'-methoxyisoflavonoids. Formononetin, 2',7-dihydroxy- and 7-hydroxy-4'-methoxyisoflavanone, and 2',7-dihydroxy-4'-methoxyisoflavone were all good precursors of I, II, sativan, and vestitol, and thus a metabolic grid may be involved in their biosynthetic origin.

IT **71815-41-3P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 71815-41-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-[4-(methoxy-14C)phenyl]-(9CI) (CA INDEX NAME)



L39 ANSWER 47 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1979:148432 HCAPLUS

DOCUMENT NUMBER: 90:148432

TITLE: Isoflavonoid constituents of Dalbergia and Machaerium species. Part 3. Vestitol and vesticarpan, isoflavonoids from Machaerium vestitum

AUTHOR(S): Kurosawa, Kazu; Ollis, W. David; Redman, Brian T.; Sutherland, Ian O.; Gottlieb, Otto R.

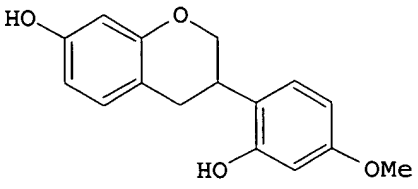
CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, UK

SOURCE: Phytochemistry (Elsevier) (1978), 17(8), 1413-15
CODEN: PYTCAS; ISSN: 0031-9422

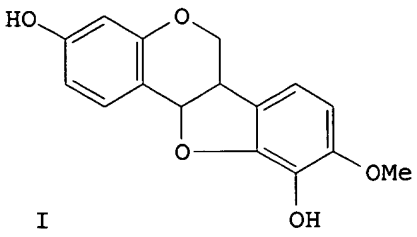
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



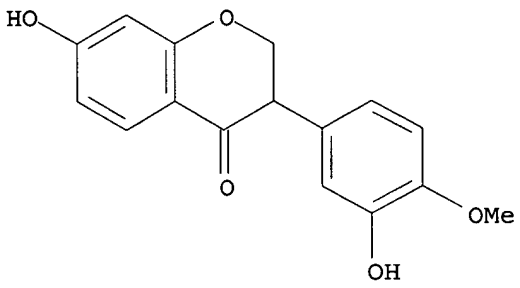
II

AB (+)-Vestitol (I) and (+)-vesticarpan (II) were isolated from the trunkwood of M. vestitum. Also isolated were O-acetyloleanolic aldehyde, formononetin, (+)-medicarpin, and (-)-mucronulatol. The structures of I and II were detd. by chem. and spectral means.

IT **67492-31-3P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 67492-31-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(3-hydroxy-4-methoxyphenyl)-(9CI) (CA INDEX NAME)



L39 ANSWER 48 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1979:54856 HCAPLUS

DOCUMENT NUMBER: 90:54856

TITLE: Synthesis of bryacarpene 3 and bryacarpene 5

AUTHOR(S): Ahluwalia, V. K.; Prakash, Chandra; Rani, Nimmi

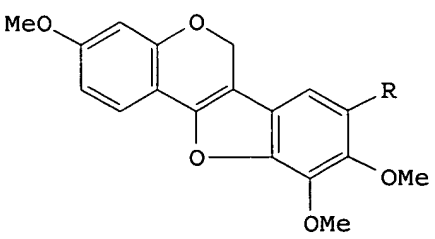
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(5), 372-4
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



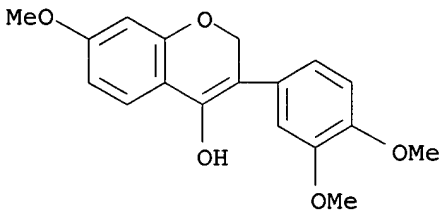
I

AB Bryacarpene 3 (I, R = MeO) was prepd. from 3,4,5-trimethoxyphenylacetonitrile and resorcinol in 6 steps. Bryacarpene 5 (I, R = H) was prepd. from 2,3,4-trimethoxybenzaldehyde and hippuric acid in 17 steps.

IT **68750-02-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of)

RN 68750-02-7 HCAPLUS

CN 2H-1-Benzopyran-4-ol, 3-(3,4-dimethoxyphenyl)-7-methoxy- (9CI) (CA INDEX NAME)



L39 ANSWER 49 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1978:503700 HCAPLUS

DOCUMENT NUMBER: 89:103700

TITLE: The chemistry of Brazilian Leguminosae. Part 55. Isoflavonoids from Myroxylon balsamum

AUTHOR(S): De Oliveira, Alaide B.; Madruga, M. Iracema L. M.; Gottlieb, Otto R.

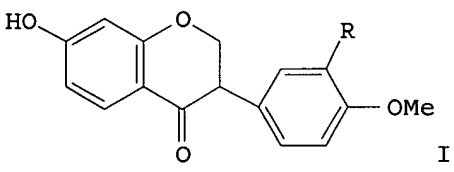
CORPORATE SOURCE: Inst. Cienc. Exatas, Univ. Fed. Minas Gerais, Belo Horizonte, Brazil

SOURCE: Phytochemistry (Elsevier) (1978), 17(3), 593-5
CODEN: PYTCAS; ISSN: 0031-9422

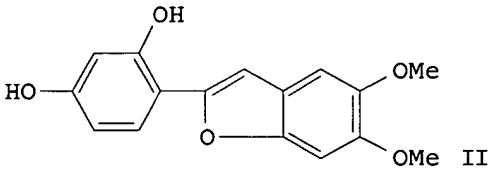
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

AB The structures of isoflavones I (R = H, OH) and of benzofuran II, isolated from M. balsamum, were detd. spectroscopically.

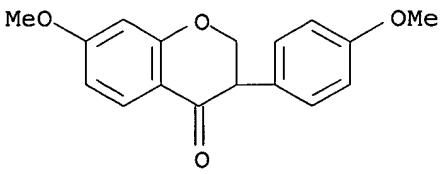
IT **67492-32-4P 67492-35-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of, isoflavone by)

RN 67492-32-4 HCAPLUS

RN 67492-35-7 HCAPLUS

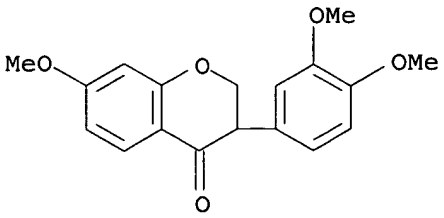
L39 ANSWER 50 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1978:136409 HCAPLUS
DOCUMENT NUMBER: 88:136409
TITLE: Catalytic hydrogenation of isoflavones. The preparation of (.+-.)-equol and related isoflavans
AUTHOR(S): Lamberton, John A.; Suares, Hector; Watson, Keith G.
CORPORATE SOURCE: Div. Appl. Org. Chem., CSIRO, Melbourne, Australia
SOURCE: Australian Journal of Chemistry (1978), 31(2), 455-7
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hydrogenation of daidzein, or preferably its O,O-diacetyl deriv., gives (.+-.)-equol in good yield only over Pd/C prepd according to the Wessely and Prillinger method (1939), whereas other Pd/C catalysts give mixts. of products. Hydrogenation of O,O,O-triacetylgenistein can be used to prep. isoflavin-4',5,7-triol.
IT **66036-38-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 66036-38-2 HCAPLUS

L39 ANSWER 51 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1975:479032 HCAPLUS
DOCUMENT NUMBER: 83:79032
TITLE: Hydroborations. New synthesis of O-methylformonoetin, formononetin, cabreuvin, and (+-) O-dimethylequol
AUTHOR(S): Kirkiacharian, Berdj S.; Chidiac, Henri
CORPORATE SOURCE: Lab. Pharm. Chim., Fac. Fr. Med. Pharm., Beirut, Lebanon
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1975), 280(11), 775-8
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB Isoflavones I (R = OMe, OH, OAc, R1 = H; R = R1 = OMe) were prepd. by condensing 3-RC6H4OH (R = OMe, OCH2Ph) with 3,4-R1(MeO)C6H3CH(CO2Et)2 to give II, hydroboration-chromate oxidn. of II to III (X = O, H2) and dehydrogenation of III (X = O). The dehydrogenation of III (X = O, R = OCH2Ph, R1 = H) occurred with debenzylation.
IT **15236-11-0P 56407-05-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydrogenation of)
RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

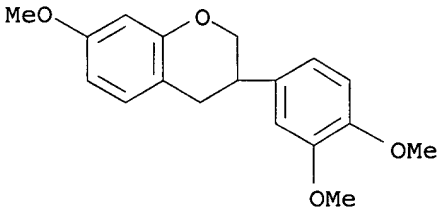


RN 56407-05-7 HCAPLUS

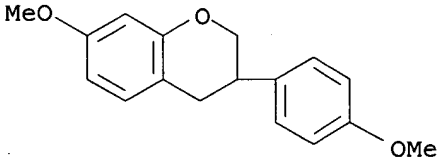
CN 4H-1-Benzopyran-4-one, 3-(3,4-dimethoxyphenyl)-2,3-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



IT **4278-54-0P 4366-35-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 4278-54-0 HCAPLUS
CN 2H-1-Benzopyran, 3-(3,4-dimethoxyphenyl)-3,4-dihydro-7-methoxy- (9CI) (CA INDEX NAME)

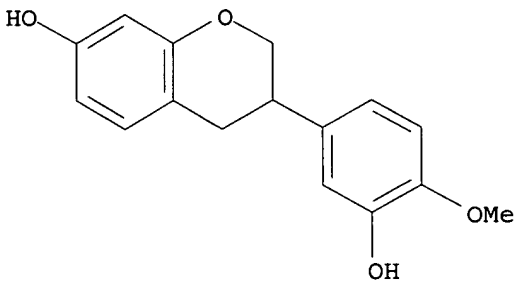


RN 4366-35-2 HCAPLUS
CN 2H-1-Benzopyran, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

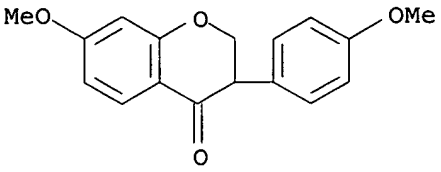


L39 ANSWER 52 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1974:120700 HCAPLUS
DOCUMENT NUMBER: 80:120700
TITLE: Synthesis of sophorol, violanone, lonchocarpan, claussequinone, philenopteran, leiocalycin, and other natural isoflavonoids by the oxidative rearrangement of chalcones with thallium(III) nitrate
AUTHOR(S): Farkas, Lorand; Gottsegen, Agnes; Nogradi, Mihaly; Antus, Sandor
CORPORATE SOURCE: Res. Group Alkaloid Chem., Hung. Acad. Sci., Budapest, Hung.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1974), (2), 305-12

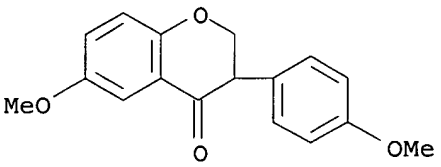
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Cyclization of 1-(2-hydroxyphenyl)-3,3-dimethoxy-2-phenylpropan-1-ones, prepd. by oxidative rearrangement of 2'-hydroxy- and -acetoxychalcones with Tl(NO3)3 in MeOH, gave, after the appropriate modifications, the title compds. E.g., (.+-.)-sophorol (I) was prepd. in 5 steps from the chalcone (II) via the isoflavone (III). Acid-catalyzed cyclization of 1-(2-hydroxy-4-methoxyphenyl)-2- 2-hydroxy-4,5-(methylenedioxy)phenyl%-3, 3-dimethoxypropan-1-one gave benzofurobenzopyrans.
IT **52250-37-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 52250-37-0 HCAPLUS
CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(3-hydroxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



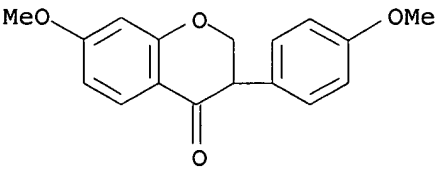
L39 ANSWER 53 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:453139 HCAPLUS
DOCUMENT NUMBER: 79:53139
TITLE: Palladium-catalyzed arylation of 4-chromanone enol esters. New synthesis of isoflavanones
AUTHOR(S): Saito, Ryuichi; Izumi, Taeko; Kasahara, Akira
CORPORATE SOURCE: Fac. Eng., Yamagata Univ., Yonezawa, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(6), 1776-9
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The Heck reaction of 4-chromanone enol esters with arylpalladium compds. in HOAc afforded iosflavanones(I) in a high yield. The structural elucidation of these products was accomplished by spectral examn.
IT **15236-11-0P 42327-66-2P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 42327-66-2 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-6-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

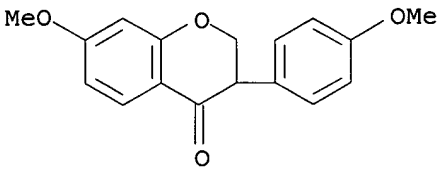


L39 ANSWER 54 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:58198 HCAPLUS
DOCUMENT NUMBER: 78:58198
TITLE: New synthesis of isoflavanones
AUTHOR(S): Aggarwal, S. K.; Grover, S. K.; Seshadri, T. R.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, India
SOURCE: Indian Journal of Chemistry (1972), 10(8), 804-7
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 3-Hydroxydeoxybenzoins were treated with CH2I2 and K2CO3 in boiling Me2CO soln. to give 12 isoflavanones.
IT **15236-11-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

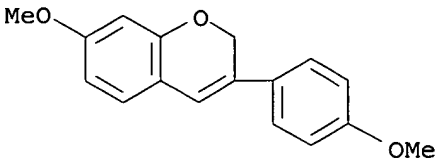


L39 ANSWER 55 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:12489 HCAPLUS
DOCUMENT NUMBER: 72:12489
TITLE: Novel synthesis of isoflavanones
AUTHOR(S): Aggarwal, S. K.; Grover, S. K.; Seshadri, Tiruvenkata R.
CORPORATE SOURCE: Univ. Delhi, Delhi, India
SOURCE: Indian Journal of Chemistry (1969), 7(10), 1059-60

CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The action of CH2I2 in the presence of Me2CO and K2CO3 on o-hydroxydeoxybenzoins yields isoflavanones. It is necessary to protect all free OH groups, except at the 2-position. The method is capable of general application as shown by the prepn. of 7-benzyloxy- (I), 4',7-dimethoxy- (II), and 5,7-dimethoxyisoflavanones (III) starting resp. from 2-hydroxy-4-benzyloxy-, 2-hydroxy-4,4'-dimethoxy-, and 2-hydroxy-4,6-dimethoxydeoxybenzoins.
IT **15236-11-0P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 15236-11-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

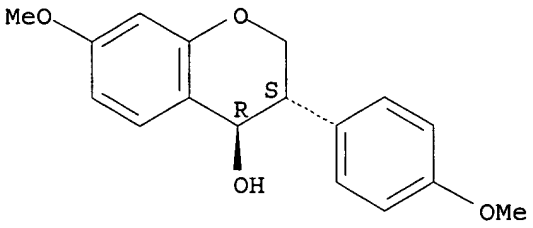


L39 ANSWER 56 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1969:11493 HCAPLUS
DOCUMENT NUMBER: 70:11493
TITLE: Syntheses of trans-isoflavan-4-ols
AUTHOR(S): Yamaguchi, Shozo; Ito, Shoei; Suzuki, Ikuko; Inoue, Naoto
CORPORATE SOURCE: Tohoku Univ., Sendai, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1968), 41(9), 2073-7
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The reaction of nitrous acid and three 4-aminoisoflavan hydrochlorides (I, II, and III) obtained by the catalytic hydrogenation of isoflavanone oximes, and the hydroboration of 3 isoflavenes (IV, V, and VI), were investigated in the hope of finding a general method of synthesizing trans-isoflavan-4-ols. The reaction of I and II with nitrous acid afforded the corresponding trans-4-ols, though in a poor yield, but that of III produced no expected compd., the corresponding isoflavene VI being obtained instead. The hydroboration of IV, V, and VI afforded the corresponding trans-alcs. (VII, VIII, and IX) in good yields. In addn., it became clear that 4-aminoisoflavans obtained by the catalytic redn. of the oximino compds. possess the 3,4-cis configuration.
IT **4308-53-6P 20986-82-7P 20986-83-8P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 4308-53-6 HCAPLUS
CN 2H-1-Benzopyran, 7-methoxy-3-(p-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)



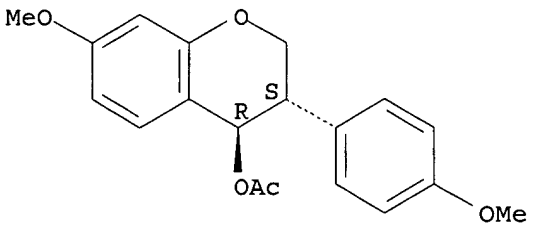
RN 20986-82-7 HCAPLUS
CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 20986-83-8 HCAPLUS
CN 4-Isoflavanol, 4',7-dimethoxy-, acetate, trans- (8CI) (CA INDEX NAME)

Relative stereochemistry.



L39 ANSWER 57 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1968:459042 HCAPLUS
DOCUMENT NUMBER: 69:59042
TITLE: Optically active aromatic chromophores. VIII. The isoflavanoid and rotenoid series
AUTHOR(S): Verbit, L.; Clark-Lewis, J. W.
CORPORATE SOURCE: State Univ. of New York, Binghamton, NY, USA
SOURCE: Tetrahedron (1968), 24(16), 5519-27
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB (-)-Equol di-Me ether (I) (4',7-dimethoxyisoflavan) is shown from O.R.D. and circular dichroism (CD) data to have the 3S-configuration instead of the R-configuration previously assigned (H. Suginome, 1966) from the plain dispersion curves at longer wavelength. The CD spectra of (-)-dihydrodeoxyrotenone and (-)-dihydrodeoxydeguelin are closely similar and their pos. Cotton effects at longer wavelength are opposite in sign to the long wavelength Cotton effects of 3S-(-)-3',4',5,7-tetramethoxyisoflavan and 3S-(-)-equol di-Me ether. The CD curves of

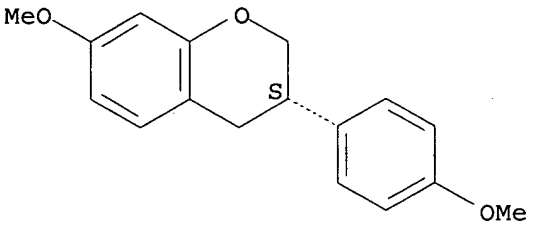
S-(+)-1-(1,4-dimethoxyphenyl)-2-(4-methoxyphenyl)propane and of S-(+)-(2,4,6-trimethoxyphenyl)-2-(3,4-dimethoxyphenyl)propane are virtually identical, and this confirms the identity in configuration of the 2 propanes previously inferred from the sign of rotation at the Na D-line, and provides a correlation of the abs. configurations of (+)-catechin, the related isoflavans, and (-)-angolensin. 16 references.

IT **3722-56-3P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

RN 3722-56-3 HCAPLUS

CN 2H-1-Benzopyran, 3,4-dihydro-7-methoxy-3-(4-methoxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L39 ANSWER 58 OF 59 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1967:443637 HCAPLUS

DOCUMENT NUMBER: 67:43637

TITLE: Flavonoids. IV. A novel Clemmensen reduction. The direct conversion of 2-alkylisoflavones to 2-alkyl-3-isoflavenes

AUTHOR(S): Dudley, Kenneth H.; Miller, H. Wayne; Corley, Robert C.; Wall, Monroe E.

CORPORATE SOURCE: Res. Triangle Inst., Durham, NC, USA

SOURCE: Journal of Organic Chemistry (1967), 32(7), 2317-21
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

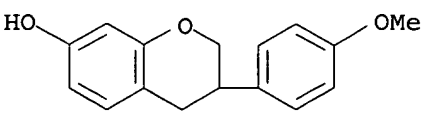
LANGUAGE: English

AB cf. preceding abstr. During a study of methods applicable to the exhaustive redn. of 2-alkylisoflavone systems, the Clemmensen redn. resulted in a direct conversion of 2-alkyl-isoflavones to 2 alkyl-3-isoflavenes. Redn. of a 2-unsubstituted isoflavone gave an isoflavene characterized as a mixt. of 2- and 3-isomers. The light absorption properties of 3-isoflavenes are discussed. 13 references.

IT **10499-17-9P 10535-63-4P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)

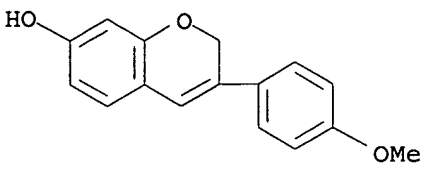
RN 10499-17-9 HCAPLUS

CN 2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 10535-63-4 HCAPLUS

CN 2H-1-Benzopyran-7-ol, 3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L39 ANSWER 59 OF 59 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:443636 HCAPLUS
DOCUMENT NUMBER: 67:43636
TITLE: Flavonoids. III. Studies on the synthesis of 2,4-dialkyl-7-acetoxy-4-methoxy-3-isoflavenes
AUTHOR(S): Dudley, Kenneth H.; Corley, Robert C.; Miller, H. Wayne; Wall, Monroe E.
CORPORATE SOURCE: Res. Triangle Inst., Durham, NC, USA
SOURCE: Journal of Organic Chemistry (1967), 32(7), 2312-17
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 64: 3464a. A method is described for the conversion of 2-methyl-7-tetrahydropyranyloxy-4'-methoxy-isoflavone to 2-methyl-4-alkyl - 7 - acetoxy - 4' -methoxy - 3 - isoflavenes (I). The incorporation of the tetrahydropyranyloxy group, as contrasted with alkyl ether groups, permits a facile cleavage of the protecting group (required for the borohydride redn. step) at a later stage in the synthesis. The synthesis entails the steps: 7-tetrahydropyranyloxyisoflavone .fwdarw. [7-tetrahydropyranyloxyisoflavanol] .fwdarw. 7 - tetrahydropyranyloxyisoflavanone .fwdarw. [4-alkyl-7-tetrahydropyranyloxyisoflavanol] .fwdarw. [4-alkyl-7-hydroxy-3-isoflavene] .fwdarw. 4-alkyl- 7 - acetoxy - 3-isoflavene. 21 references.
IT **4626-22-6P**
RL: **SPN (Synthetic preparation)**; PREP (Preparation)
(prepn. of)
RN 4626-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)